

**A VARIATIONAL FORMULATION FOR MODELING A
PROTIUM HYDROGEN MOLECULAR IONIZATION**

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Abstract

This article develops a variational formulation for modeling a protium hydrogen molecular ionization obtained through a high temperature scalar field and an appropriate electric one action. The results are based on standard tools of calculus of variations and optimization theory. Finally, we highlight the context here addressed is essentially an Euler-Bernoullian one and includes the establishment of a new approximate Bernoulli-interacting-gas type equation.

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1 Introduction

The first part of this article develops a variational formulation for modeling the ionization of a gaseous hydrogen molecular system, through a high temperature field and an appropriate electric field. The context here developed is an Euler-Bernoullian one.

Such results are based on tools of calculus of variations and related Lagrange multipliers approach.

It is worth emphasizing we have obtained a new system of partial differential equations for modeling a compressible case in fluid mechanics, similar to those found in the contemporary literature however, with a new Bernoullian-interacting-gas equation replacing a standard ideal gas equation and related interacting one, in such a concerning model. A related similar result for a simpler case may be found in [1].

We also highlight the two main fields for such a system are a position one and a velocity one, which we specify below in the next lines.

As standard references in theoretical fluid mechanics we would cite [2, 3, 4, 5, 6]. For related numerical methods we would mention [7, 8, 9, 10]. Concerning similar models, we would cite [11, 12, 13, 14, 15, 16].

Finally, details on the Sobolev spaces involved may be found in [17].

2 A note on the first Maxwell equation of electromagnetism

Firstly, we highlight the main results in this section have been previously presented in similar form in the Preprint [18].

Let $\Omega_1 \subset \mathbb{R}^3$ be an open, bounded and connected set with a regular (Lipschitzian) boundary denoted by $\partial\Omega_1$.

Suppose $\mathbf{E} : \Omega_1 \rightarrow \mathbb{R}^3$ is an electric field of resulting from a punctual charge q localized at $(0, 0, 0) \in \Omega_1$.

Let $\Omega \subset \Omega_1$ be also an open, bounded and connected set with a regular (C^1 class) boundary denoted by $S = \partial\Omega$, such that $(0, 0, 0) \in \Omega$, where, in polar coordinates $(r, \theta, \phi) \in \mathbb{R}^3$, we have

$$S = \{\mathbf{r}(\theta, \phi) : 0 \leq \theta \leq \pi \text{ and } 0 \leq \phi \leq 2\pi\},$$

and where,

$$\mathbf{r}(\theta, \phi) = X(\theta, \phi)\mathbf{i} + Y(\theta, \phi)\mathbf{j} + Z(\theta, \phi)\mathbf{k}.$$

and

$$\mathbf{i} = (1, 0, 0), \mathbf{j} = (0, 1, 0), \mathbf{k} = (0, 0, 1) \in \mathbb{R}^3.$$

Observe that denoting

$$\mathbf{e}_r = \sin(\theta) \cos(\phi) \mathbf{i} + \sin(\theta) \sin(\phi) \mathbf{j} + \cos(\theta) \mathbf{k},$$

we have

$$\mathbf{E} = \hat{K} q \frac{1}{r^2} \mathbf{e}_r,$$

for an appropriate real constant $\hat{K}$.

We highlight the integral

$$I_n = \int_S \mathbf{E} \cdot \mathbf{n} \, dS = c_5$$

where such a real constant c_5 does not depend on the C^1 class function

$$\mathbf{r} : [0, \pi] \times [0, 2\pi] \rightarrow \mathbb{R}^3.$$

Here $\mathbf{n}$ denotes the normal outward field to S .

In this section, we develop such an integral I_n , in details.

Denoting

$$R(\theta, \phi) = \|\mathbf{r}(\theta, \phi)\|_{\mathbb{R}^3},$$

we have

$$\mathbf{r}(\theta, \phi) = R(\theta, \phi) \mathbf{e}_r.$$

Moreover, we recall that

$$dS = \|\mathbf{r}_\theta \times \mathbf{r}_\phi\|_{\mathbb{R}^3} \, d\theta d\phi,$$

where

$$N = \mathbf{r}_\theta \times \mathbf{r}_\phi$$

is such that

$$\mathbf{n} = \frac{N}{\|N\|_{\mathbb{R}^3}}.$$

Thus

$$\int_S \mathbf{E} \cdot \mathbf{n} \, dS = \hat{K} q \int_{\phi=0}^{\phi=2\pi} \int_{\theta=0}^{\theta=\pi} \frac{1}{R(\theta, \phi)^2} \mathbf{e}_r \cdot \frac{N}{\|N\|_{\mathbb{R}^3}} \|N\|_{\mathbb{R}^3} \, d\theta d\phi.$$

In summary,

$$\int_S \mathbf{E} \cdot \mathbf{n} \, dS = \hat{K} q \int_{\phi=0}^{\phi=2\pi} \int_{\theta=0}^{\theta=\pi} \frac{1}{R(\theta, \phi)^2} \mathbf{e}_r \cdot N \, d\theta \, d\phi.$$

Observe that

$$\begin{aligned}
 N &= (R(\theta, \phi) \mathbf{e}_r)_\theta \times (R(\theta, \phi) \mathbf{e}_r)_\phi \\
 &= (R_\theta \mathbf{e}_r + R(\mathbf{e}_r)_\theta) \times (R_\phi \mathbf{e}_r + R(\mathbf{e}_r)_\phi) \\
 &= R_\theta R_\phi \mathbf{e}_r \times \mathbf{e}_r + R_\theta \mathbf{e}_r \times R(\mathbf{e}_r)_\phi \\
 &\quad + R(\mathbf{e}_r)_\theta \times (R_\phi \mathbf{e}_r) + R^2(\mathbf{e}_r)_\theta \times (\mathbf{e}_r)_\phi.
 \end{aligned} \tag{1}$$

Consequently, from such results, we obtain

$$\mathbf{e}_r \cdot N = R^2 \mathbf{e}_r \cdot (\mathbf{e}_r)_\theta \times (\mathbf{e}_r)_\phi.$$

Thus, we have got

$$\begin{aligned}
 &\int_S \mathbf{E} \cdot \mathbf{n} \, dS \\
 &= \hat{K} q \int_{\phi=0}^{\phi=2\pi} \int_{\theta=0}^{\theta=\pi} \frac{1}{R(\theta, \phi)^2} \mathbf{e}_r \cdot N \, d\theta \, d\phi \\
 &= \hat{K} q \int_{\phi=0}^{\phi=2\pi} \int_{\theta=0}^{\theta=\pi} \frac{1}{R(\theta, \phi)^2} R(\theta, \phi)^2 \mathbf{e}_r \cdot (\mathbf{e}_r)_\theta \times (\mathbf{e}_r)_\phi \, d\theta \, d\phi \\
 &= \hat{K} q \, 4\pi \\
 &\equiv c_5.
 \end{aligned} \tag{2}$$

Summarizing, we have got

$$\int_S \mathbf{E} \cdot \mathbf{n} \, dS = c_5.$$

where such a real constant does not depend on function $\mathbf{r} : [0, \pi] \times [0, 2\pi] \rightarrow \mathbb{R}^3$.

Consider now a charge q_0 localized at the center of a sphere Ω_2 of radius $R > 0$ and boundary $S_2 = \partial\Omega_2$.

The electric field on the sphere surface generated by q_0 is given by

$$\mathbf{E}_2 = \frac{1}{4\pi\epsilon_0} \frac{q_0}{R^2} \mathbf{n}_2,$$

where $\mathbf{n}_2$ is the normal outward field to S_2 .

Clearly

$$\int_{S_2} \mathbf{E}_2 \cdot \mathbf{n}_2 \, dS_2 = \frac{1}{4\pi\epsilon_0} \frac{q_0}{R^2} (4\pi R^2) = \frac{q_0}{\epsilon_0}.$$

Consider again the set Ω but now with a charge q_0 localized at a point $\mathbf{x}$ inside the interior of Ω , which is denoted by Ω^0 .

At first the electric field $\mathbf{E}$ generated by q_0 is not of C^1 class on Ω .

However, there exists $R > 0$ such that

$$B_R(\mathbf{x}) \subset \Omega = \Omega^0.$$

Define $\Omega_3 = \Omega \setminus B_R(\mathbf{x})$.

Therefore, $\mathbf{E}$ is of C^1 class on Ω_3 .

Denoting the boundary of Ω_3 by $S_3 = \partial\Omega \cup \partial B_R(\mathbf{x})$, from the previous results and denoting again $S = \partial\Omega$, we may infer that

$$\int_{S_3} \mathbf{E} \cdot \mathbf{n} dS_3 = \int_S \mathbf{E} \cdot \mathbf{n} dS - \int_{\partial B_R(\mathbf{x})} \mathbf{E} \cdot \mathbf{n} dS_2 = c_5 - c_5 = 0,$$

for a not relabeled real constant c_5 , so that

$$\begin{aligned} \int_{S_3} \mathbf{E} \cdot \mathbf{n} dS_3 &= \int_S \mathbf{E} \cdot \mathbf{n} dS - \int_{\partial B_R(\mathbf{x})} \mathbf{E} \cdot \mathbf{n} dS_2 \\ &= \int_S \mathbf{E} \cdot \mathbf{n} dS - \frac{q_0}{\varepsilon_0} \\ &= 0. \end{aligned} \tag{3}$$

Therefore, we have got

$$\int_S \mathbf{E} \cdot \mathbf{n} dS = \frac{q_0}{\varepsilon_0}.$$

Assume now on Ω we have a density of charges $\rho(\mathbf{x})$.

For a small volume $\Delta\tilde{V}$ consider a punctual charge q_0 localized in $\mathbf{x} \in \Omega$ such that

$$q_0 \approx \rho(\mathbf{x})\Delta\tilde{V}.$$

Denoting by $\Delta\mathbf{E}$ the electric field generated by q_0 , from the previous results we may infer that

$$\int_S \Delta\mathbf{E} \cdot \mathbf{n} dS = \frac{q_0}{\varepsilon_0} \approx \frac{\rho(\mathbf{x})\Delta\tilde{V}}{\varepsilon_0}.$$

Such an equation in its differential form, stands for:

$$\int_S d\mathbf{E} \cdot \mathbf{n} dS = \frac{\rho(\mathbf{x}) d\tilde{V}}{\varepsilon_0}.$$

Integrating in Ω we may obtain

$$\begin{aligned}\int_S \mathbf{E} \cdot \mathbf{n} dS &= \int_S \int_{\Omega} d\mathbf{E} \cdot \mathbf{n} dS \\ &= \int_{\Omega} \frac{\rho(\mathbf{x})}{\varepsilon_0} d\tilde{V},\end{aligned}\tag{4}$$

so that

$$\int_S \mathbf{E} \cdot \mathbf{n} dS = \int_{\Omega} \frac{\rho(\mathbf{x})}{\varepsilon_0} d\tilde{V}.$$

From this and the Divergence Theorem, we have

$$\int_S \mathbf{E} \cdot \mathbf{n} dS = \int_{\Omega} \operatorname{div} \mathbf{E} d\tilde{V} = \int_{\Omega} \frac{\rho(\mathbf{x})}{\varepsilon_0} d\tilde{V}.$$

Summarizing, we have got

$$\int_{\Omega} \operatorname{div} \mathbf{E} d\tilde{V} = \int_{\Omega} \frac{\rho(\mathbf{x})}{\varepsilon_0} d\tilde{V}.$$

This is the integral form of the first Maxwell equation of electromagnetism.

For this last equation, the set $\Omega \subset \Omega_1$ is rather arbitrary so that for Ω as a ball of small radius $r > 0$ with center at a point $\mathbf{x} \in \Omega_1$, from the Mean Value Theorem for integrals and letting $r \rightarrow 0^+$, we obtain

$$\operatorname{div} \mathbf{E} = \frac{\rho}{\varepsilon_0}, \text{ in } \Omega_1.$$

This last equation stands for the differential form of the first Maxwell equation of electromagnetism.

Remark 2.1. Summarizing, in this section we have formally obtained a mathematical deduction of the first Maxwell equation of electromagnetism.

Remark 2.2. Suppose beyond the electric field $\mathbf{E}$ generated by a charge density ρ , we have an external one associated with an external electric C^1 class potential V .

Hence, the total electric field, here denoted by $\mathbf{E}_{total}$, is given by

$$\mathbf{E}_{total} = \mathbf{E} - \nabla V.$$

Hence

$$\mathbf{E} = \mathbf{E}_{total} + \nabla V,$$

so that from the previous results obtained, we have

$$\operatorname{div} \mathbf{E} = \operatorname{div} (\mathbf{E}_{total} + \nabla V) = \frac{\rho}{\varepsilon_0}.$$

Finally, considering other unit systems, we may find in the literature also the following expression for this first Maxwell equation:

$$\operatorname{div} \mathbf{E} = 4\pi\rho.$$

3 About a first variational formulation for compressible fluid mechanics including electromagnetic fields

Let $\Omega \subset \mathbb{R}^3$ be an open, bounded and simply connected set with a regular (Lipschitzian) boundary denoted by $\partial\Omega$.

Generically, we consider a fluid motion initially modeled as a particle system one, through the field of position $\mathbf{r} : \Omega \times [0, T] \rightarrow \mathbb{R}^3$ and field of velocities $\mathbf{v}$ where $\mathbf{v}(\mathbf{r}(x, t), t)$ stands for the velocity at the position $\mathbf{r}(x, t)$ and time $t \in [0, T]$.

Consider a functional J which represents a variational formulation for such a motion, where

$$\begin{aligned} J(\mathbf{r}, \mathbf{v}, \rho) = & \frac{1}{2} \int_0^T \int_{\Omega} \rho(\mathbf{r}(x, t), t) \mathbf{v}(\mathbf{r}(x, t), t) \cdot \mathbf{v}(\mathbf{r}(x, t), t) \, dx dt \\ & + \int_0^T \int_{\Omega} \lambda \left(\mathbf{v}(\mathbf{r}(x, t), t) - \frac{\partial \mathbf{r}(x, t)}{\partial t} \right) \, dx dt \\ & - \int_0^T \int_{\Omega} \hat{P} \left(\frac{d\rho}{dt} + \rho \operatorname{div} (\mathbf{v}) \right) \, dx dt \\ & - \int_0^T \int_{\Omega} \rho \mathbf{g} \cdot \mathbf{r} \, dx dt \end{aligned} \quad (5)$$

Here we have generically denoted

$$\rho = \rho(\mathbf{r}(x, t), t),$$

$$\mathbf{v} = \mathbf{v}(\mathbf{r}(x, t), t),$$

and

$$\mathbf{r} = \mathbf{r}(x, t).$$

In a second step, for an electronic field, we include electric and magnetic fields

and associated potentials in such a variational formulation, obtaining

$$\begin{aligned}
 J_1(\mathbf{r}, \mathbf{v}, \rho, \mathbf{A}, V) &= J(\mathbf{r}, \mathbf{v}, \rho) - K_1 \int_0^T \int_{\Omega} \rho \mathbf{A} \cdot \frac{\partial \mathbf{r}(x, t)}{\partial t} dx dt \\
 &\quad - K_1 \int_0^T \int_{\Omega} V(\mathbf{r}) \rho dx dt + \frac{1}{8\pi} \| \text{Curl } \mathbf{A} - \mathbf{B}_0 \|_{0,2,\Omega \times [0,T]}^2 \\
 &\quad - \frac{1}{8\pi} \left\| \nabla V + \frac{1}{c} \frac{\partial \mathbf{A}}{\partial t} \right\|_{0,2,\Omega \times [0,T]}^2 \\
 &\quad - \int_0^T \int_{\Omega} \rho \mathbf{B}(x, t) \times \frac{\partial \mathbf{r}(x, t)}{\partial t} \cdot (\mathbf{r}(\varepsilon t, x) - (\mathbf{r}_0)(x)) dx dt \\
 &= \frac{1}{2} \int_0^T \int_{\Omega} \rho(\mathbf{r}(x, t), t) \mathbf{v}(\mathbf{r}(x, t), t) \cdot \mathbf{v}(\mathbf{r}(x, t), t) dx dt \\
 &\quad + \int_0^T \int_{\Omega} \lambda \left(\mathbf{v}(\mathbf{r}(x, t), t) - \frac{\partial \mathbf{r}(x, t)}{\partial t} \right) dx dt \\
 &\quad - \int_0^T \int_{\Omega} \hat{P} \left(\frac{d\rho}{dt} + \rho \text{div}(\mathbf{v}) \right) dx dt \\
 &\quad - \int_0^T \int_{\Omega} \rho \mathbf{g} \cdot \mathbf{r} dx dt \\
 &\quad - K_1 \int_0^T \int_{\Omega} \rho \mathbf{A} \cdot \frac{\partial \mathbf{r}(x, t)}{\partial t} dx dt \\
 &\quad - K_1 \int_0^T \int_{\Omega} V(\mathbf{r}) \rho dx dt + \frac{1}{8\pi} \| \text{Curl } \mathbf{A} - \mathbf{B}_0 \|_{0,2,\Omega \times [0,T]}^2 \\
 &\quad - \frac{1}{8\pi} \left\| \nabla V + \frac{1}{c} \frac{\partial \mathbf{A}}{\partial t} \right\|_{0,2,\Omega \times [0,T]}^2 \\
 &\quad - \int_0^T \int_{\Omega} \rho \mathbf{B}(x, t) \times \frac{\partial \mathbf{r}(x, t)}{\partial t} \cdot (\mathbf{r}(\varepsilon t, x) - (\mathbf{r}_0)(x)) dx dt \quad (6)
 \end{aligned}$$

where,

$$\mathbf{B} = \mathbf{B}_0 - \text{Curl } \mathbf{A}$$

is the total magnetic field, $\mathbf{B}_0$ is an external magnetic field and $\mathbf{A} = (A_1, A_2, A_3)$ is the magnetic potential,

$$V(\mathbf{r})$$

is the electric potential and

$$\mathbf{E} = \nabla V + \frac{1}{c} \frac{\partial \mathbf{A}}{\partial t},$$

is the electric field.

From the variation of J_1 in $\mathbf{v}$, we have

$$\rho \mathbf{v} + \lambda + \nabla(\rho \hat{P}) = \mathbf{0},$$

$\in \Omega \times [0, T]$.

From the variation of P in ρ , we obtain

$$\frac{1}{2} \mathbf{v} \cdot \mathbf{v} + \frac{d\hat{P}}{dt} - \hat{P} \operatorname{div}(\mathbf{v}) + K_1 \mathbf{A} \cdot \frac{\partial \mathbf{r}}{\partial t} + K_1 V - \mathbf{g} \cdot \mathbf{r} = 0,$$

$\in \Omega \times [0, T]$.

From the variation of J_1 in $\mathbf{r}$, we obtain

$$\begin{aligned} \frac{dJ_1}{d\mathbf{r}} &= \frac{\partial J_1}{\partial \mathbf{v}} \frac{\partial \mathbf{v}}{\partial \mathbf{r}} \\ &\quad + \frac{\partial J_1}{\partial \rho} \frac{\partial \rho}{\partial \mathbf{r}} \\ &\quad + \frac{\partial J_1}{\partial \mathbf{A}} \frac{\partial \mathbf{A}}{\partial \mathbf{r}} \\ &\quad + \frac{\partial J_1}{\partial V} \frac{\partial V}{\partial \mathbf{r}} + \frac{\partial J_1}{\partial \mathbf{r}} \\ &= \frac{\partial J_1}{\partial \mathbf{r}} \\ &= \mathbf{0}. \end{aligned} \tag{7}$$

Such a Gâteaux differential

$$\frac{dJ_1}{d\mathbf{r}}$$

is related to the following variation of J_1 in $\mathbf{r}$, which lead us to the correct Euler-Lagrange equation,

$$\begin{aligned} \left\langle \frac{dJ_1}{d\mathbf{r}}, \varphi \right\rangle_{L^2} &= \hat{\delta}(J_1)_{\mathbf{r}}(\mathbf{r}, \mathbf{r}(\varepsilon t, x), \mathbf{v}, \rho, \mathbf{A}, V; \varphi) \\ &= \lim_{h \rightarrow 0} [J_1(\mathbf{r} + h\varphi, \mathbf{r}(\varepsilon t, x) + h\varphi, \mathbf{v}, \rho, \mathbf{A}, V) \\ &\quad - J_1(\mathbf{r}, \mathbf{r}(\varepsilon t, x), \mathbf{v}, \rho, \mathbf{A}, V)] / h \\ &= \mathbf{0}, \quad \forall \varphi \in C_c^\infty(\Omega \times [0, T]; \mathbb{R}^3). \end{aligned} \tag{8}$$

The corresponding Euler-Lagrange equation stands for,

$$\frac{\partial \lambda}{\partial t} - \rho \mathbf{g} + K_1 \frac{\partial(\rho \mathbf{A})}{\partial t} - K_1 \rho \mathbf{B} \times \mathbf{v} + \mathcal{O}(\varepsilon) = \mathbf{0},$$

in $\Omega \times [0, T]$.

From the variation of J_1 in $\hat{P}$, we have

$$\frac{d\rho}{dt} + \rho \operatorname{div}(\mathbf{v}) = 0,$$

Consequently, from such previous results, letting $\varepsilon \rightarrow 0^+$, we obtain

$$\begin{aligned} 0 &= \frac{\partial \lambda}{\partial t} - \rho \mathbf{g} + K_1 \frac{\partial(\rho \mathbf{A})}{\partial t} - K_1 \rho \mathbf{B} \times \mathbf{v} \\ &= -\frac{d(\rho \mathbf{v})}{dt} - \frac{d\nabla(\rho \hat{P})}{dt} \\ &\quad - \rho \mathbf{g} + K_1 \frac{\partial(\rho \mathbf{A})}{\partial t} \\ &\quad - K_1 \rho \mathbf{B} \times \mathbf{v}. \end{aligned} \tag{9}$$

Now defining $P = \frac{d(\rho \hat{P})}{dt}$, we obtain

$$\begin{aligned} &\frac{d(\rho \mathbf{v})}{dt} + \nabla P \\ &\quad + \rho \mathbf{g} - K_1 \frac{\partial(\rho \mathbf{A})}{\partial t} + K_1 \rho \mathbf{v} \times \mathbf{B} \\ &= 0, \end{aligned} \tag{10}$$

in $\Omega \times [0, T]$.

Observe that

$$\begin{aligned} P &= \frac{d(\rho \hat{P})}{dt} \\ &= \frac{d\rho}{dt} \hat{P} + \rho \frac{d\hat{P}}{dt}. \end{aligned} \tag{11}$$

Thus,

$$\frac{P}{\rho} = \frac{d\rho}{dt} \frac{\hat{P}}{\rho} + \frac{d\hat{P}}{dt},$$

so that

$$\begin{aligned} \frac{P}{\rho} &= \frac{d\rho}{dt} \frac{\hat{P}}{\rho} - \frac{1}{2} \mathbf{v} \cdot \mathbf{v} + K_1 \mathbf{A} \cdot \frac{\partial \mathbf{r}}{\partial t} - K_1 V + \mathbf{g} \cdot \mathbf{r} + \hat{P} \operatorname{div}(\mathbf{v}) \\ &= \left(\frac{d\rho}{dt} + \rho \operatorname{div}(\mathbf{v}) \right) \frac{\hat{P}}{\rho} - \frac{1}{2} \mathbf{v} \cdot \mathbf{v} + K_1 \mathbf{A} \cdot \frac{\partial \mathbf{r}}{\partial t} - K_1 V + \mathbf{g} \cdot \mathbf{r} \\ &= -\frac{1}{2} \mathbf{v} \cdot \mathbf{v} + K_1 \mathbf{A} \cdot \frac{\partial \mathbf{r}}{\partial t} - K_1 V + \mathbf{g} \cdot \mathbf{r}. \end{aligned} \tag{12}$$

Therefore, we have obtained the Bernoulli type equation

$$\frac{P}{\rho} + \frac{1}{2} \mathbf{v} \cdot \mathbf{v} - \mathbf{g} \cdot \mathbf{r} = K_1 \mathbf{A} \cdot \frac{\partial \mathbf{r}}{\partial t} - K_1 V.$$

Remark 3.1. Observe that the variation of J in V stands for

$$K_1\rho - \frac{1}{4\pi} \operatorname{div} \left(\nabla V + \frac{1}{c} \frac{\partial \mathbf{A}}{\partial t} \right) = 0.$$

Hence, recalling that

$$\mathbf{E} = \nabla V + \frac{1}{c} \frac{\partial \mathbf{A}}{\partial t},$$

we have obtained

$$\operatorname{div} \mathbf{E} = 4\pi K_1\rho.$$

Considering the statements in remark 2.2, we have that such an electric field $\mathbf{E}$ is the one exclusively generated by the density ρ so that, also from such a remark, we have

$$\mathbf{E} = \mathbf{E}_{total} + \nabla V = \nabla V + \frac{1}{c} \frac{\partial \mathbf{A}}{\partial t}.$$

Thus, from such results, the total electric field stands for

$$E_{total} = \frac{1}{c} \frac{\partial \mathbf{A}}{\partial t}.$$

Hence, for a time independent ρ , the associated total electric field force density stands for

$$\mathbf{f}_e = -K_1 \frac{\rho}{c} \frac{\partial \mathbf{A}}{\partial t},$$

where, in atomic units, we have $c = 1$, so that

$$\mathbf{f}_e = -K_1 \rho \frac{\partial \mathbf{A}}{\partial t}.$$

Moreover, the density force associated with the magnetic field is given by

$$\mathbf{f}_m = K_1 \rho \mathbf{v} \times \mathbf{B},$$

so that

$$\mathbf{f}_e + \mathbf{f}_m = -K_1 \frac{\rho}{c} \frac{\partial \mathbf{A}}{\partial t} + K_1 \rho \mathbf{v} \times \mathbf{B}.$$

Indeed for a time dependent density, we have found the following Euler equation as an equilibrium one,

$$\begin{aligned} & \frac{d(\rho \mathbf{v})}{dt} + \nabla P \\ & + \rho \mathbf{g} - K_1 \frac{\partial(\rho \mathbf{A})}{\partial t} + K_1 \rho \mathbf{v} \times \mathbf{B} \\ & = \mathbf{0}, \end{aligned} \tag{13}$$

in $\Omega \times [0, T]$.

Considering the statements in remark 2.2, such an equation agrees with the previous theoretical results obtained in the contemporary literature.

Remark 3.2. We are assuming ε_0 is a real constant. In a more general context we may consider a variable

$$\varepsilon_0 = \varepsilon_0(\rho(\mathbf{r}(x, t)), \mathbf{r}(x, t)).$$

In such a case, it is necessary to replace the functional part in atomic units

$$J_7 = -\frac{1}{2} \left\| \nabla V + \frac{1}{c} \frac{\partial \mathbf{A}}{\partial t} \right\|_{0,2}^2 = -\frac{1}{2} \|\mathbf{E}\|_{0,2}^2,$$

by

$$\hat{J}_7 = -\frac{1}{2} \int_0^T \int_{\Omega} \varepsilon_0(\rho(\mathbf{r}(x, t)), \mathbf{r}) \mathbf{E} \cdot \mathbf{E} \, dx dt$$

where

$$\mathbf{E} = \nabla V + \frac{1}{c} \frac{\partial \mathbf{A}}{\partial t}.$$

In such a case the final expression for the extremal equation

$$\frac{\partial J_1}{\partial \mathbf{r}}$$

would stand for

$$\begin{aligned} & \frac{d(\rho \mathbf{v})}{dt} + \nabla P \\ & + \rho \mathbf{g} - K_1 \frac{\partial(\rho \mathbf{A})}{\partial t} + K_1 \rho \mathbf{v} \times \mathbf{B} \\ & + \frac{1}{2} \frac{d\varepsilon_0(\rho(\mathbf{r}), \mathbf{r})}{d\mathbf{r}} \mathbf{E} \cdot \mathbf{E}. \\ & = 0, \end{aligned} \tag{14}$$

in $\Omega \times [0, T]$.

4 A note on the Energy equation

We define the power function P_w by

$$P_w = \left\{ -\frac{\partial J_2}{\partial \mathbf{r}} \cdot \frac{\partial \mathbf{r}}{\partial t} : \text{subject to } \frac{\partial J_2}{\partial \mathbf{v}} = \frac{\partial J_2}{\partial \mathbf{A}} = \mathbf{0} \text{ and } \frac{\partial J_2}{\partial \rho} = \frac{\partial J_2}{\partial V} = 0 \right\}.$$

where

$$\begin{aligned} & J_2(\mathbf{r}, \mathbf{v}, \rho, \mathbf{A}, V) \\ = & \frac{1}{2} \int_0^T \int_{\Omega} \rho(\mathbf{r}(x, t), t) \mathbf{v}(\mathbf{r}(x, t), t) \cdot \mathbf{v}(\mathbf{r}(x, t), t) \, dx dt \\ & + \int_0^T \int_{\Omega} \lambda_1 \left(\mathbf{v}(\mathbf{r}(x, t), t) - \frac{\partial \mathbf{r}(x, t)}{\partial t} \right) \, dx dt + \int_0^T \int_{\Omega} \rho \mathbf{g} \cdot \mathbf{r} \, dx dt \\ & - K_1 \int_0^T \int_{\Omega} \rho \mathbf{A} \cdot \frac{\partial \mathbf{r}(x, t)}{\partial t} \, dx dt \\ & - K_1 \int_0^T \int_{\Omega} V(\mathbf{r}) \rho \, dx dt + \frac{1}{8\pi} \| \text{Curl } \mathbf{A} - \mathbf{B}_0 \|_{0,2,\Omega \times [0,T]}^2 \\ & - \frac{1}{8\pi} \left\| \nabla V + \frac{1}{c} \frac{\partial \mathbf{A}}{\partial t} \right\|_{0,2,\Omega \times [0,T]}^2 \\ & - K_1 \int_0^T \int_{\Omega} \rho \mathbf{B}(x, t) \times \frac{\partial \mathbf{r}(x, t)}{\partial t} \cdot (\mathbf{r}(\varepsilon t, x) - (\mathbf{r}_0)(x)) \, dx dt. \end{aligned} \quad (15)$$

Such a Gâteaux differential

$$\frac{dJ_2}{d\mathbf{r}}$$

is related to the following variation of J_2 in $\mathbf{r}$, which lead us to the correct Euler-Lagrange equation,

$$\begin{aligned} & \left\langle \frac{dJ_2}{d\mathbf{r}}, \varphi \right\rangle_{L^2} = \hat{\delta}(J_2)_{\mathbf{r}}(\mathbf{r}, \mathbf{r}(\varepsilon t, x), \mathbf{v}, \rho, \mathbf{A}, V; \varphi) \\ = & \lim_{h \rightarrow 0} [J_2(\mathbf{r} + h\varphi, \mathbf{r}(\varepsilon t, x) + h\varphi, \mathbf{v}, \rho, \mathbf{A}, V) \\ & - J_2(\mathbf{r}, \mathbf{r}(\varepsilon t, x), \mathbf{v}, \rho, \mathbf{A}, V)] / h \\ = & \mathbf{0}, \quad \forall \varphi \in C_c^\infty(\Omega \times [0, T]; \mathbb{R}^3). \end{aligned} \quad (16)$$

The corresponding Euler-Lagrange equation stands for,

$$\frac{\partial \lambda_1}{\partial t} - \rho \mathbf{g} + K_1 \frac{\partial(\rho \mathbf{A})}{\partial t} - K_1 \rho \mathbf{B} \times \mathbf{v} + \mathcal{O}(\varepsilon) = \mathbf{0},$$

in $\Omega \times [0, T]$.

With such a result and the restriction

$$\frac{\partial J_2}{\partial \mathbf{v}} = \mathbf{0},$$

which stands for

$$(\rho \mathbf{v}) + \lambda_1 = \mathbf{0},$$

so that from this and $P = \frac{d(\rho \hat{P})}{dt}$, we obtain

$$P_w = \left(\frac{d(\rho \mathbf{v})}{dt} + \rho \mathbf{g} - K_1 \frac{\partial(\rho \mathbf{A})}{\partial t} + K_1 \rho \mathbf{B} \times \mathbf{v} \right) \cdot \mathbf{v} \quad (17)$$

in $\Omega \times [0, T]$.

Moreover, for an infinitesimal block volume $\tilde{V}$ of dimensions Δx_1 , Δx_2 and Δx_3 located at $(x_1, x_2, x_3, t) \in \Omega \times [0, T]$, we define for the pressure P , the following power variation,

$$\begin{aligned} \Delta \dot{W}_1 &= ((Pv_1)(x_1 + \Delta x_1, x_2, x_3, t) - (Pv_1)(x_1, x_2, x_3, t)) \Delta x_2 \Delta x_3 \\ &\quad + ((Pv_2)(x_1, x_2 + \Delta x_2, x_3, t) - (Pv_2)(x_1, x_2, x_3, t)) \Delta x_1 \Delta x_3 \\ &\quad + ((Pv_3)(x_1, x_2, x_3 + \Delta x_3, t) - (Pv_3)(x_1, x_2, x_3, t)) \Delta x_1 \Delta x_2 \\ &\approx \left(\frac{\partial(Pv_1)}{\partial x_1} + \frac{\partial(Pv_2)}{\partial x_2} + \frac{\partial(Pv_3)}{\partial x_3} \right) \Delta x_1 \Delta x_2 \Delta x_3 \\ &= \operatorname{div}(P\mathbf{v}) \Delta x_1 \Delta x_2 \Delta x_3. \end{aligned} \quad (18)$$

Also, concerning the temperature effects, denoting the temperature field by T_e , we generically assume the Fourier Law,

$$\dot{Q} = KA \frac{\partial T_e}{\partial \mathbf{n}},$$

for a general flat area A with a surface normal outward field denoted by $\mathbf{n}$.

Here $\dot{Q}$ denotes the heat flux through A in a direction normal to A .

Concerning our elementary small volume $\tilde{V}$, we define the following heat variation $\Delta \dot{Q}$, where

$$\begin{aligned} \Delta \dot{Q} &= K_e \left(\frac{\partial T_e}{\partial x_1}(x_1 + \Delta x_1, x_2, x_3, t) - \frac{\partial T_e}{\partial x_1}(x_1, x_2, x_3) \right) \Delta x_2 \Delta x_3 \\ &\quad + K_e \left(\frac{\partial T_e}{\partial x_2}(x_1, x_2 + \Delta x_2, x_3, t) - \frac{\partial T_e}{\partial x_2}(x_1, x_2, x_3) \right) \Delta x_1 \Delta x_3 \\ &\quad + K_e \left(\frac{\partial T_e}{\partial x_3}(x_1, x_2, x_3 + \Delta x_3, t) - \frac{\partial T_e}{\partial x_3}(x_1, x_2, x_3) \right) \Delta x_1 \Delta x_2 \\ &\approx K_e \left(\frac{\partial^2 T_e}{\partial x_1^2} + \frac{\partial^2 T_e}{\partial x_2^2} + \frac{\partial^2 T_e}{\partial x_3^2} \right) \Delta x_1 \Delta x_2 \Delta x_3 \\ &= K_e \nabla^2 T_e \Delta x_1 \Delta x_2 \Delta x_3. \end{aligned} \quad (19)$$

for some appropriate real constant $K_e > 0$.

Finally, for the Power variation concerning the internal variables, we define

$$E_{in} = \frac{1}{2} \rho \frac{d\mathbf{r}_e}{dt} \cdot \frac{d\mathbf{r}_e}{dt},$$

where generically

$$\mathbf{r}_e = \mathbf{r}_e(\mathbf{r}(x, t), t),$$

refers to a internal energy displacement field.

Moreover, we set the restriction,

$$C_v T_e = \frac{1}{2} \frac{d\mathbf{r}_e}{dt} \cdot \frac{d\mathbf{r}_e}{dt}, \text{ in } \Omega \times [0, T].$$

Observe that

$$-\frac{dE_{in}}{d\mathbf{r}_e} \cdot \frac{d\mathbf{r}_e}{dt} = \frac{d\left(\rho \frac{d\mathbf{r}_e}{dt}\right)}{dt} \cdot \frac{d\mathbf{r}_e}{dt}. \quad (20)$$

Now assuming

$$\left| \frac{d\rho}{dt} \frac{d\mathbf{r}_e}{dt} \right| \ll \left| \rho \frac{d^2(\mathbf{r}_e)}{dt^2} \right|,$$

we obtain

$$\begin{aligned} -\frac{dE_{in}}{d\mathbf{r}_e} \cdot \frac{d\mathbf{r}_e}{dt} &= \frac{d\left(\rho \frac{d\mathbf{r}_e}{dt}\right)}{dt} \cdot \frac{d\mathbf{r}_e}{dt} \\ &\approx \rho \frac{d^2(\mathbf{r}_e)}{dt^2} \cdot \frac{d\mathbf{r}_e}{dt} \\ &= \frac{\rho}{2} \frac{d\left(\frac{d\mathbf{r}_e}{dt} \cdot \frac{d\mathbf{r}_e}{dt}\right)}{dt} \\ &= \rho \frac{d(C_v T_e)}{dt}. \end{aligned} \quad (21)$$

Denoting

$$\Delta P_{in} = \rho \frac{d(C_v T_e)}{dt} \Delta x_1 \Delta x_2 \Delta x_3,$$

from an application of the First Law of Thermodynamics for such an elementary volume $\tilde{V}$, we have

$$P_w \Delta x_1 \Delta x_2 \Delta x_3 + \Delta P_{in} \approx -\Delta \dot{W} + \Delta \dot{Q}.$$

Therefore, we have obtained

$$\begin{aligned}
 & P_w + \rho \frac{d(C_v T_e)}{dt} \\
 & \approx -\operatorname{div}(P \mathbf{v}) + K_e \nabla^2 T_e \\
 & = -\nabla P \cdot \mathbf{v} - P \operatorname{div} \mathbf{v} + K_e \nabla^2 T_e.
 \end{aligned} \tag{22}$$

Now observe that

$$P_w + \nabla P \cdot \mathbf{v} = \left(\frac{d(\rho \mathbf{v})}{dt} + \nabla P + \rho \mathbf{g} - K_1 \frac{\partial(\rho \mathbf{A})}{\partial t} + K_1 \rho \mathbf{B} \times \mathbf{v} \right) \cdot \mathbf{v} = 0,$$

so that, we have got

$$\rho \frac{d(C_v T_e)}{dt} = K_e \nabla^2 T_e - P \operatorname{div} \mathbf{v}.$$

which is a standard energy equation found in the fluid mechanics books, for an inviscid compressible case.

Remark 4.1. *Generically, for an ideal gas, we will define the entropy function by*

$$S = -K_B \frac{\rho}{\rho_0} \ln \left(\frac{\rho}{e \rho_0} \right),$$

where ρ is the gas density field, ρ_0 is a reference density field, $K_B > 0$ is an appropriate real constant and e is the natural exponential basis.

Observe that for an ideal gas, we have

$$P = R \rho T_e,$$

where P is the pressure field, T_e is the temperature one and $R > 0$ is an appropriate constant.

From such results and definitions, we obtain,

$$\begin{aligned}
 S &= -K_B \frac{\rho}{\rho_0} \ln \left(\frac{\rho}{e \rho_0} \right) \\
 &= -K_B \frac{\rho}{\rho_0} \ln \left(\frac{P}{e R T_e \rho_0} \right) \\
 &= -K_B \frac{\rho}{\rho_0} \ln \left(\frac{P R T_0}{e R T_e P_0} \right) \\
 &= -K_B \frac{\rho}{\rho_0} \ln \left(\frac{P}{e P_0} \frac{T_0}{T_e} \right) \\
 &= -K_B \frac{\rho}{\rho_0} \ln \left(\frac{P}{e P_0} \right) + K_B \frac{\rho}{\rho_0} \ln \left(\frac{T_e}{T_0} \right)
 \end{aligned} \tag{23}$$

This final formula is similar to those found in the standard physics undergraduate books.

Including such an entropy function part

$$E_S = T_e S,$$

we obtain the final form of the energy equation,

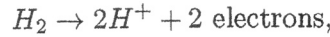
$$\rho \frac{d(C_v T_e)}{dt} = K_e \nabla^2 T_e - P \operatorname{div} \mathbf{v} + \frac{dE_S}{dt}.$$

The objective of this section is complete.

5 On the ionization chemical reaction and the corresponding plasma generation

In this section, we develop in details the concerning variational formulation for a compressible case.

We emphasize such a set $\Omega \subset \mathbb{R}^3$ stands for a control volume, in which along a time interval $[0, T]$, where $t \in [0, T]$ denotes time, a gaseous hydrogen molecular system will be ionized, through its exposition to a high scalar temperature field and an appropriate electric one, as it is indicated in the following reaction equation



generating a corresponding plasma.

We recall that a hydrogen (protium) molecule is comprised by two hydrogen (protium) atoms, with an electron and one proton each one (no neutrons).

5.1 The mathematical model

Denoting by m_e, m_p the masses of one electron and one proton, respectively, we start by defining the following hydrogen molecular density

$$\begin{aligned} \hat{\rho}_{H_2}(x, y, z, t) &= (|\phi_{e_1}(x, y, z, t)|^2 + |\phi_{p_1}(x, y, z, t)|^2) \\ &\quad \times \frac{|\phi_{A_1}(y, z, t)|^2}{2m_e + 2m_p} \rho_{H_2}(z, t) \\ &\quad + (|\phi_{e_2}(x, y, z, t)|^2 + |\phi_{p_2}(x, y, z, t)|^2) \\ &\quad \times \frac{|\phi_{A_2}(y, z, t)|^2}{2m_e + 2m_p} \rho_{H_2}(z, t). \end{aligned} \tag{24}$$

The corresponding ion densities $\hat{\rho}_{H_a^+}$ and $\hat{\rho}_{H_b^+}$ are defined by

$$\begin{aligned}\hat{\rho}_{H_a^+}(x, y, z, t) &= (|\phi_{p_3}(x, y, z, t)|^2) \\ &\times |\phi_{A_3}(y, z, t)|^2 \frac{\rho_{H_a^+}(z, t)}{m_p}\end{aligned}\quad (25)$$

and

$$\begin{aligned}\hat{\rho}_{H_b^+}(x, y, z, t) &= (|\phi_{p_4}(x, y, z, t)|^2) \\ &\times |\phi_{A_4}(y, z, t)|^2 \frac{\rho_{H_b^+}(z, t)}{m_p}\end{aligned}\quad (26)$$

In this text, we consider ρ_{H_2} , $\rho_{H_a^+}$, $\rho_{H_b^+}$, ϕ_{H_2} , $\phi_{H_a^+}$ and $\phi_{H_b^+}$ as independent variables which satisfy the following restrictions,

$$\rho_{H_2}(z, t) = |\phi_{H_2}(z, t)|^2.$$

$$\rho_{H_a^+}(z, t) = |\phi_{H_a^+}(z, t)|^2,$$

and

$$\rho_{H_b^+}(z, t) = |\phi_{H_b^+}(z, t)|^2,$$

respectively.

For the free electronic fields resulting from such an ionization, we denote

$$\rho_{e_3}(z, t) = |\phi_{e_3}(z, t)|^2,$$

and

$$\rho_{e_4}(z, t) = |\phi_{e_4}(z, t)|^2,$$

$$\rho_e(z, t) = \rho_{e_3}(z, t) + \rho_{e_4}(z, t).$$

Moreover, we denote

$$\hat{\rho}_{e_1}(x, y, z, t) = (|\rho_{e_1}(x, y, z, t)|^2) |\phi_{A_1}(y, z, t)|^2 \frac{|\phi_{H_2}(z, t)|^2}{2m_e + 2m_p},$$

$$\hat{\rho}_{e_2}(x, y, z, t) = (|\phi_{e_2}(x, y, z, t)|^2) |\phi_{A_2}(y, z, t)|^2 \frac{|\phi_{H_2}(z, t)|^2}{2m_e + 2m_p},$$

$$\hat{\rho}_{p_1}(x, y, z, t) = (|\phi_{p_1}(x, y, z, t)|^2) |\phi_{A_1}(y, z, t)|^2 \frac{|\phi_{H_2}(z, t)|^2}{2m_e + 2m_p},$$

and

$$\hat{\rho}_{p_2}(x, y, z, t) = (|\phi_{p_2}(x, y, z, t)|^2) |\phi_{A_2}(y, z, t)|^2 \frac{|\phi_{H_2}(z, t)|^2}{2m_e + 2m_p},$$

$$\hat{\rho}_{p_3}(x, y, z, t) = (|\phi_{p_3}(x, y, z, t)|^2) |\phi_{A_3}(y, z, t)|^2 \frac{|\phi_{H_a^+}(z, t)|^2}{m_p},$$

$$\hat{\rho}_{p_4}(x, y, z, t) = (|\phi_{p_4}(x, y, z, t)|^2) |\phi_{A_4}(y, z, t)|^2 \frac{|\phi_{H_b^+}(z, t)|^2}{m_p},$$

$$\rho_{e_1}(z, t) = \int_{\Omega} \int_{\Omega} \hat{\rho}_{e_1}(x, y, z, t) dx dy,$$

$$\rho_{e_2}(z, t) = \int_{\Omega} \int_{\Omega} \hat{\rho}_{e_2}(x, y, z, t) dx dy,$$

$$\rho_{p_1}(z, t) = \int_{\Omega} \int_{\Omega} \hat{\rho}_{p_1}(x, y, z, t) dx dy,$$

$$\rho_{p_2}(z, t) = \int_{\Omega} \int_{\Omega} \hat{\rho}_{e_2}(x, y, z, t) dx dy,$$

$$\rho_{p_3}(z, t) = \int_{\Omega} \int_{\Omega} \hat{\rho}_{p_3}(x, y, z, t) dx dy,$$

$$\rho_{p_4}(z, t) = \int_{\Omega} \int_{\Omega} \hat{\rho}_{p_4}(x, y, z, t) dx dy.$$

Here the subscripts e_j , p_j , A_j refer to a density of electrons, protons and atoms for $j \in \{1, 2, 3, 4\}$.

We define also the following function spaces,

$$\begin{aligned} V_1 &= \{(\phi_{e_1}, \phi_{e_2}) \in W^{1,2}(\Omega \times \Omega \times \Omega \times [0, T]; \mathbb{C}^2) : \\ &\quad \nabla_x \phi_{e_j} \cdot \mathbf{n} = 0, \text{ on } \partial\Omega \times \Omega \times \Omega \times [0, T], \\ &\quad \nabla_y \phi_{e_j} \cdot \mathbf{n} = 0, \text{ on } \Omega \times \partial\Omega \times \Omega \times [0, T], \\ &\quad \nabla_z \phi_{e_j} \cdot \mathbf{n} = 0, \text{ on } \Omega \times \Omega \times \partial\Omega \times [0, T], \\ &\quad \frac{\partial \phi_{e_j}(x, y, z, 0)}{\partial t} = 0 \\ &\quad \text{and } \frac{\partial \phi_{e_j}(x, y, z, T)}{\partial t} = 0, \text{ in } \Omega \times \Omega \times \Omega, \forall j \in \{1, 2\} \}, \end{aligned} \quad (27)$$

$$\begin{aligned}
 V_2 = & \{(\phi_{p_1}, \phi_{p_2}) \in W^{1,2}(\Omega \times \Omega \times \Omega \times [0, T]; \mathbb{C}^2) : \\
 & \nabla_x \phi_{p_j} \cdot \mathbf{n} = 0, \text{ on } \partial\Omega \times \Omega \times \Omega \times [0, T], \\
 & \nabla_y \phi_{p_j} \cdot \mathbf{n} = 0, \text{ on } \Omega \times \partial\Omega \times \Omega \times [0, T], \\
 & \nabla_z \phi_{p_j} \cdot \mathbf{n} = 0, \text{ on } \Omega \times \Omega \times \partial\Omega \times [0, T], \\
 & \frac{\partial \phi_{p_j}(x, y, z, 0)}{\partial t} = 0 \\
 & \text{and } \frac{\partial \phi_{p_j}(x, y, z, T)}{\partial t} = 0, \text{ in } \Omega \times \Omega \times \Omega, \forall j \in \{1, 2\} \}, \quad (28)
 \end{aligned}$$

$$\begin{aligned}
 V_3 = & \{(\phi_{e_3}, \phi_{e_4}) \in W^{1,2}(\Omega \times [0, T]; \mathbb{C}^2) : \nabla_z \phi_{e_j} \cdot \mathbf{n} = 0, \text{ on } \partial\Omega \times [0, T], \\
 & \frac{\partial \phi_{e_j}(z, 0)}{\partial t} = 0 \text{ and } \frac{\partial \phi_{e_j}(z, T)}{\partial t} = 0, \\
 & \text{in } \Omega \times \Omega \times \Omega, \forall j \in \{3, 4\} \}, \quad (29)
 \end{aligned}$$

$$\begin{aligned}
 V_4 = & \{(\phi_{p_3}, \phi_{p_4}) \in W^{1,2}(\Omega \times \Omega \times \Omega \times [0, T]; \mathbb{C}^2) : \\
 & \nabla_x \phi_{p_j} \cdot \mathbf{n} = 0, \text{ on } \partial\Omega \times \Omega \times \Omega \times [0, T], \\
 & \nabla_y \phi_{p_j} \cdot \mathbf{n} = 0, \text{ on } \Omega \times \partial\Omega \times \Omega \times [0, T], \\
 & \nabla_z \phi_{p_j} \cdot \mathbf{n} = 0, \text{ on } \Omega \times \Omega \times \partial\Omega \times [0, T], \\
 & \frac{\partial \phi_{p_j}(x, y, z, 0)}{\partial t} = 0 \\
 & \text{and } \frac{\partial \phi_{p_j}(x, y, z, T)}{\partial t} = 0, \text{ in } \Omega \times \Omega \times \Omega, \forall j \in \{3, 4\} \}, \quad (30)
 \end{aligned}$$

$$\begin{aligned}
 V_5 = & \{(\phi_{A_1}, \phi_{A_2}) \in W^{1,2}(\Omega \times \Omega \times [0, T]; \mathbb{C}^2) : \\
 & \nabla_y \phi_{A_j} \cdot \mathbf{n} = 0, \text{ on } \partial\Omega \times \Omega \times [0, T], \\
 & \nabla_z \phi_{A_j} \cdot \mathbf{n} = 0, \text{ on } \Omega \times \partial\Omega \times [0, T], \\
 & \frac{\partial \phi_{A_j}(y, z, 0)}{\partial t} = 0 \\
 & \text{and } \frac{\partial \phi_{A_j}(y, z, T)}{\partial t} = 0, \text{ in } \Omega \times \Omega, \forall j \in \{1, 2\} \}, \quad (31)
 \end{aligned}$$

$$\begin{aligned}
 V_6 = & \left\{ (\phi_{A_3}, \phi_{A_4}) \in W^{1,2}(\Omega \times \Omega \times [0, T]; \mathbb{C}^2) : \right. \\
 & \nabla_y \phi_{A_j} \cdot \mathbf{n} = 0, \text{ on } \partial\Omega \times \Omega \times [0, T], \\
 & \nabla_z \phi_{A_j} \cdot \mathbf{n} = 0, \text{ on } \Omega \times \partial\Omega \times [0, T], \\
 & \frac{\partial \phi_{A_j}(y, z, 0)}{\partial t} = 0 \\
 & \left. \text{and } \frac{\partial \phi_{A_j}(y, z, T)}{\partial t} = 0, \text{ in } \Omega \times \Omega, \forall j \in \{3, 4\} \right\}, \quad (32)
 \end{aligned}$$

$$\begin{aligned}
 V_7 = & \left\{ (\phi_{H_2}, \phi_{H_a^+}, \phi_{H_b^+}) \in W^{1,2}(\Omega \times [0, T]; \mathbb{C}^3) : \right. \\
 & (\phi_{H_2}, \phi_{H_a^+}, \phi_{H_b^+}) = \mathbf{0} \text{ on } \partial(\Omega_1 \cup \Omega_2) \times [0, T], \\
 & (\phi_{H_2}(z, t), \phi_{H_a^+}(z, t), \phi_{H_b^+}(z, t)) = (\phi_{(H_2)_{in}}(z, t), 0, 0) \text{ on } \partial\Omega_{in} \times [0, T] \\
 & \left. \text{and } (\phi_{H_2}(z, 0), \phi_{H_a^+}(z, 0), \phi_{H_b^+}(z, 0)) = (\phi_0, 0, 0) \text{ in } \Omega \right\}, \quad (33)
 \end{aligned}$$

where

$$\partial\Omega = \partial\Omega_{in} \cup \partial\Omega_1 \cup \partial\Omega_2 \cup \partial\Omega_{out}.$$

Moreover we suppose such a union is quasi-disjoint and through $\partial\Omega_{in}$ and $\partial\Omega_{out}$ are allowed the entering and leaving of gaseous mass, respectively.

5.2 The position fields

We start by denoting the macroscopic molecular hydrogen position field as

$$\mathbf{r}_{H_2} : \Omega \times [0, T] \rightarrow \mathbb{R}^3.$$

The atomic position fields are defined by

$$\mathbf{r}_{A_j}(x, t) = \mathbf{r}_{H_2}(x, t) + \hat{\mathbf{r}}_{A_j}(\mathbf{r}_{H_2}(x, t), t),$$

for $j \in \{1, 2\}$, and

$$\mathbf{r}_{A_3}(x, t) = \mathbf{r}_{H_a^+}(x, t) + \hat{\mathbf{r}}_{A_3}(\mathbf{r}_{H_a^+}(x, t), t),$$

$$\mathbf{r}_{A_4}(x, t) = \mathbf{r}_{H_b^+}(x, t) + \hat{\mathbf{r}}_{A_4}(\mathbf{r}_{H_b^+}(x, t), t),$$

where

$$\mathbf{r}_{H_a^+} : \Omega \times [0, T] \rightarrow \mathbb{R}^4,$$

and

$$\mathbf{r}_{H_b^+} : \Omega \times [0, T] \rightarrow \mathbb{R}^4$$

denote the macroscopic ion position field for the ions H_a^+ and H_b^+ , respectively.

Moreover, in a relativistic context, for the electronic fields

$$\hat{\mathbf{r}}_{e_j}(x, t) = \mathbf{r}_{A_j}(x, t) + \tilde{\mathbf{r}}_{e_j}(\mathbf{r}_{A_j}(x, t), t) = (\mathbf{r}_{H_2}(x, t), t) + (ct, \mathbf{r}_{e_j}(\mathbf{r}_{H_2}(x, t))),$$

for $j \in \{1, 2\}$.

For the proton fields,

$$\hat{\mathbf{r}}_{p_j}(x, t) = \mathbf{r}_{A_j}(x, t) + \tilde{\mathbf{r}}_{p_j}(\mathbf{r}_{A_j}(x, t), t) = (\mathbf{r}_{H_2}(x, t), t) + (ct, \mathbf{r}_{p_j}(\mathbf{r}_{H_2}(x, t))),$$

for $j \in \{1, 2\}$.

Moreover for the ion proton fields

$$\hat{\mathbf{r}}_{p_3}(x, t) = \mathbf{r}_{A_3}(x, t) + \tilde{\mathbf{r}}_{p_3}(\mathbf{r}_{A_3}(x, t), t) = (\mathbf{r}_{H_a^+}(x, t), t) + (ct, \mathbf{r}_{p_3}(\mathbf{r}_{H_a^+}(x, t))),$$

and

$$\hat{\mathbf{r}}_{p_4}(x, t) = \mathbf{r}_{A_4}(x, t) + \tilde{\mathbf{r}}_{p_4}(\mathbf{r}_{A_4}(x, t), t) = (\mathbf{r}_{H_b^+}(x, t), t) + (ct, \mathbf{r}_{p_4}(\mathbf{r}_{H_b^+}(x, t))),$$

Here $c > 0$ denotes the speed of light.

Finally, generically we shall denote,

$$\mathbf{v}_{H_2} = \mathbf{v}_{H_2}(\mathbf{r}_{H_2}(x, t), t),$$

$$\mathbf{v}_{H_a^+} = \mathbf{v}_{H_a^+}(\mathbf{r}_{H_a^+}(x, t), t),$$

$$\mathbf{v}_{H_b^+} = \mathbf{v}_{H_b^+}(\mathbf{r}_{H_b^+}(x, t), t),$$

$$\mathbf{v}_{e_3} = \mathbf{v}_{e_3}(\mathbf{r}_{e_3}(x, t), t)$$

and

$$\mathbf{v}_{e_4} = \mathbf{v}_{e_4}(\mathbf{r}_{e_4}(x, t), t),$$

with a similar corresponding notation for the remaining particles and atoms.

Here we define the following function spaces,

$$\begin{aligned} V_8 &= \left\{ \mathbf{r} = (\mathbf{r}_{H_2}, \mathbf{r}_{H_a^+}, \mathbf{r}_{H_b^+}) \in W^{1,2}(\Omega \times [0, T]; \mathbb{R}^{3 \times 3}) : \right. \\ &\quad \mathbf{r} = \mathbf{0} \text{ on } (\partial\Omega_1 \cap \partial\Omega_2) \times [0, T] \\ &\quad \left. \text{and } \mathbf{r}(z, 0) = \mathbf{r}_0 \text{ in } \Omega \right\}, \end{aligned} \tag{34}$$

and

$$(\mathbf{r}_{e_1}, \mathbf{r}_{e_2}) \in V_9 = W^{1,2}(\mathbb{R}^3 \times [0, T]; \mathbb{R}^{4 \times 2}),$$

$$\begin{aligned}
(\mathbf{r}_{p_1}, \mathbf{r}_{p_2}) &\in V_{10} = W^{1,2}(\mathbb{R}^3 \times [0, T]; \mathbb{R}^{4 \times 2}), \\
(\mathbf{v}_{p_3}, \mathbf{v}_{p_4}) &\in V_{11} = W^{1,2}(\mathbb{R}^3 \times [0, T]; \mathbb{R}^{4 \times 2}), \\
(\mathbf{r}_{e_3}, \mathbf{r}_{e_4}) &\in V_{12} = W^{1,2}(\Omega \times [0, T]; \mathbb{R}^{4 \times 2}), \\
(\mathbf{r}_{A_1}, \mathbf{r}_{A_2}) &\in V_{13} = W^{1,2}(\mathbb{R}^3 \times [0, T]; \mathbb{R}^{3 \times 2}), \\
(\mathbf{r}_{A_3}, \mathbf{r}_{A_3}) &\in V_{14} = W^{1,2}(\mathbb{R}^3 \times [0, T]; \mathbb{R}^{3 \times 2}).
\end{aligned}$$

$$\begin{aligned}
V_{15} = \{ \mathbf{v} = (\mathbf{v}_{H_2}, \mathbf{v}_{H_a^+}, \mathbf{v}_{H_b^+}) \in W^{1,2}(\mathbb{R}^3 \times [0, T]; \mathbb{R}^{3 \times 3}) : \mathbf{v} = \mathbf{0} \text{ on } (\partial\Omega_1 \cap \partial\Omega_2) \times [0, T] \\
\text{and } \mathbf{v}(\mathbf{r}, 0) = \mathbf{v}_0 \text{ in } \Omega \}, \tag{35}
\end{aligned}$$

and

$$\begin{aligned}
(\mathbf{v}_{e_1}, \mathbf{v}_{e_2}) &\in V_{16} = W^{1,2}(\mathbb{R}^3 \times [0, T]; \mathbb{R}^{4 \times 2}), \\
(\mathbf{v}_{p_1}, \mathbf{v}_{p_2}) &\in V_{17} = W^{1,2}(\mathbb{R}^3 \times [0, T]; \mathbb{R}^{4 \times 2}), \\
(\mathbf{v}_{p_3}, \mathbf{v}_{p_4}) &\in V_{18} = W^{1,2}(\mathbb{R}^3 \times [0, T]; \mathbb{R}^{4 \times 2}), \\
(\mathbf{v}_{e_3}, \mathbf{v}_{e_4}) &\in V_{19} = W^{1,2}(\Omega \times [0, T]; \mathbb{R}^{4 \times 2}), \\
(\mathbf{v}_{A_1}, \mathbf{v}_{A_2}) &\in V_{20} = W^{1,2}(\mathbb{R}^3 \times [0, T]; \mathbb{R}^{3 \times 2}), \\
(\mathbf{v}_{A_3}, \mathbf{v}_{A_3}) &\in V_{21} = W^{1,2}(\mathbb{R}^3 \times [0, T]; \mathbb{R}^{3 \times 2}).
\end{aligned}$$

5.3 About the system constraints

Denoting by $m_{H_2}(0)$ the total system mass at $t = 0$, we have the following constraint

$$\begin{aligned}
m_{H_2}(0) &= \int_{\Omega} \rho_{H_2}(z, 0) dz \\
&= \int_{\Omega} \rho_{H_2}(z, t) dz + \int_0^t \int_{\partial\Omega} \rho_{H_2}(z, \tau) \mathbf{v}_{H_2} \cdot \mathbf{n} dS d\tau \\
&\quad + \int_{\Omega} \rho_{H_a^+}(z, t) dz + \int_0^t \int_{\partial\Omega} \rho_{H_a^+}(z, \tau) \mathbf{v}_{H_a^+} \cdot \mathbf{n} dS d\tau \\
&\quad + \int_{\Omega} \rho_{H_b^+}(z, t) dz + \int_0^t \int_{\partial\Omega} \rho_{H_b^+}(z, \tau) \mathbf{v}_{H_b^+} \cdot \mathbf{n} dS d\tau \\
&\quad + \int_{\Omega} \rho_{e_3}(z, t) dz + \int_0^t \int_{\partial\Omega} \rho_{e_3}(z, \tau) \mathbf{v}_{e_3} \cdot \mathbf{n} dS d\tau \\
&\quad + \int_{\Omega} \rho_{e_4}(z, t) dz + \int_0^t \int_{\partial\Omega} \rho_{e_4}(z, \tau) \mathbf{v}_{e_4} \cdot \mathbf{n} dS d\tau \tag{36}
\end{aligned}$$

We have also the following constraint

$$\begin{aligned} & \int_{\Omega} \rho_{e_3}(z, t) dz + \int_0^t \int_{\partial\Omega} \rho_{e_3}(z, \tau) \mathbf{v}_{e_3} \cdot \mathbf{n} dS d\tau \\ &= \int_{\Omega} \rho_{e_4}(z, t) dz + \int_0^t \int_{\partial\Omega} \rho_{e_4}(z, \tau) \mathbf{v}_{e_4} \cdot \mathbf{n} dS d\tau \end{aligned} \quad (37)$$

Here $\mathbf{n}$ denotes the outward normal field to $\partial\Omega = S$.

Relating the kinetics energy, we define the following functionals

$$\begin{aligned} E_{C_1} &= -\frac{1}{2} \int_0^T \int_{\Omega} \frac{\rho_{e_1}(z, t)}{\sqrt{1 - \frac{v_{e_1}^2}{c^2}}} \frac{d\tilde{\mathbf{r}}_{e_1}}{dt} \cdot \frac{d\tilde{\mathbf{r}}_{e_1}}{dt} \sqrt{-g^{e_1}} |\det X'_{H_2}| dz dt \\ &= \frac{1}{2} \int_0^T \int_{\Omega} \frac{\rho_{e_1}(z, t)}{\sqrt{1 - \frac{v_{e_1}^2}{c^2}}} (c^2 - v_{e_1}^2) \sqrt{-g^{e_1}} |\det X'_{H_2}| dz dt \\ &= \frac{1}{2} \int_0^T \int_{\Omega} c \rho_{e_1}(z, t) \sqrt{c^2 - v_{e_1}^2} \sqrt{-g^{e_1}} |\det X'_{H_2}| dz dt \\ &= \frac{1}{2} \int_0^T \int_{\Omega} c \rho_{e_1}(z, t) \sqrt{c^2 - g_{jk}^{e_1} \frac{\partial(X_{H_2})_j}{\partial t} \frac{\partial(X_{H_2})_k}{\partial t}} \sqrt{-g^{e_1}} |\det X'_{H_2}| dz dt, \end{aligned}$$

where generically, we have denoted, $X_0 = t$,

$$g_{jk}^{e_1} = \frac{\partial \mathbf{r}_{e_1}}{\partial (X_{H_2})_j} \cdot \frac{\partial \mathbf{r}_{e_1}}{\partial (X_{H_2})_k}$$

$g^{e_1} = \det\{g_{jk}^{e_1}\}$, where

$$a \cdot b = -a_0 b_0 + \sum_{k=1}^3 a_k b_k$$

for

$$a = (a_0, a_1, a_2, a_3)$$

and

$$b = (b_0, b_1, b_2, b_3) \in \mathbb{R}^4.$$

Similarly, we may define

$$E_{C_2} = \frac{1}{2} \int_0^T \int_{\Omega} c \rho_{p_1}(z, t) \sqrt{c^2 - g_{jk}^{p_1} \frac{\partial(X_{H_2})_j}{\partial t} \frac{\partial(X_{H_2})_k}{\partial t}} \sqrt{-g^{p_1}} |\det X'_{H_2}| dz dt \quad (38)$$

and also,

$$E_{C_3} = \frac{1}{2} \int_0^T \int_{\Omega} c \rho_{e_2}(z, t) \sqrt{c^2 - g_{jk}^{e_2} \frac{\partial(X_{H_2})_j}{\partial t} \frac{\partial(X_{H_2})_k}{\partial t}} \sqrt{-g^{e_2}} |\det X'_{H_2}| dz dt \quad (39)$$

Furthermore, we may define

$$E_{C_4} = \frac{1}{2} \int_0^T \int_{\Omega} c \rho_{p_2}(z, t) \sqrt{c^2 - g_{jk}^{p_2} \frac{\partial(X_{H_2})_j}{\partial t} \frac{\partial(X_{H_2})_k}{\partial t}} \sqrt{-g^{p_2}} |\det X'_{H_2}| dz dt \quad (40)$$

Similarly, for the ions particles

$$E_{C_5} = \frac{1}{2} \int_0^T \int_{\Omega} c \rho_{p_3}(z, t) \sqrt{c^2 - g_{jk}^{p_3} \frac{\partial(X_{H_a^+})_j}{\partial t} \frac{\partial(X_{H_a^+})_k}{\partial t}} \sqrt{-g^{p_3}} |\det X'_{H_a^+}| dz dt \quad (41)$$

$$E_{C_6} = \frac{1}{2} \int_0^T \int_{\Omega} c \rho_{p_4}(z, t) \sqrt{c^2 - g_{jk}^{p_4} \frac{\partial(X_{H_b^+})_j}{\partial t} \frac{\partial(X_{H_b^+})_k}{\partial t}} \sqrt{-g^{p_4}} |\det X'_{H_b^+}| dz dt \quad (42)$$

$$E_{C_7} = \frac{1}{2} \int_0^T \int_{\Omega} c \rho_{e_3}(z, t) \sqrt{c^2 - v_{e_3}^2} \sqrt{-g^{e_3}} dz dt, \quad (43)$$

$$E_{C_8} = \frac{1}{2} \int_0^T \int_{\Omega} c \rho_{e_4}(z, t) \sqrt{c^2 - v_{e_4}^2} \sqrt{-g^{e_4}} dz dt. \quad (44)$$

For the interacting and self-interacting energies, in a non-linear Schrödinger equation context, we define the following functionals,

$$\begin{aligned}
E_{in} = & \frac{\alpha_1}{2} \int_0^T \int_{\Omega} \int_{\Omega} \int_{\Omega} |\hat{\rho}_{H_2}(x, y, z, t)|^2 dx dy dz dt \\
& + \frac{\alpha_2}{2} \int_0^T \int_{\Omega} \int_{\Omega} \int_{\Omega} |\hat{\rho}_{H_a^+}(x, y, z, t)|^2 dx dy dz dt \\
& + \frac{\alpha_3}{2} \int_0^T \int_{\Omega} \int_{\Omega} \int_{\Omega} |\hat{\rho}_{H_b^+}(x, y, z, t)|^2 dx dy dz dt \\
& + \frac{\alpha_4}{2} \int_0^T \int_{\Omega} |\rho_{e_3}(z, t)|^2 dz dt \\
& + \frac{\alpha_5}{2} \int_0^T \int_{\Omega} |\rho_{e_4}(z, t)|^2 dz dt \\
& - \frac{\beta_1}{2} \int_0^T \int_{\Omega} \int_{\Omega} \int_{\Omega} \hat{\rho}_{H_2}(x, y, z, t) dx dy dz dt \\
& - \frac{\beta_2}{2} \int_0^T \int_{\Omega} \int_{\Omega} \int_{\Omega} \hat{\rho}_{H_a^+}(x, y, z, t) dx dy dz dt \\
& - \frac{\beta_3}{2} \int_0^T \int_{\Omega} \int_{\Omega} \int_{\Omega} \hat{\rho}_{H_b^+}(x, y, z, t) dx dy dz dt \\
& - \frac{\beta_4}{2} \int_0^T \int_{\Omega} \rho_{e_3}(z, t) dz dt \\
& - \frac{\beta_5}{2} \int_0^T \int_{\Omega} \rho_{e_4}(z, t) dz dt,
\end{aligned} \tag{45}$$

On the other hand, for the terms involving the magnetic potential, we define

$$\begin{aligned}
E_{M_1} = & \frac{1}{2} \int_0^T \int_{\Omega} \int_{\Omega} \int_{\Omega} \left(\left(\frac{\gamma_1}{2m_e + 2m_p} |\nabla \phi_{e_1}(x, y, z, t) - i\rho_1 \mathbf{A}(z, t) \phi_{e_1}(x, y, z, t)|^2 \right. \right. \\
& + \frac{\gamma_2}{2m_e + 2m_p} |\nabla \phi_{p_1}(x, y, z, t) - i\rho_2 \mathbf{A}(z, t) \phi_{p_1}(x, y, z, t)|^2 \Big) \\
& \times |\phi_{A_1}(y, z, t)|^2 |\phi_{H_2}(z, t)|^2 \\
& + \left(\frac{\gamma_4}{2m_e + 2m_p} |\nabla \phi_{e_2}(x, y, z, t) - i\rho_4 \mathbf{A}(z, t) \phi_{e_2}(x, y, z, t)|^2 \right. \\
& + \frac{\gamma_5}{2m_e + 2m_p} |\nabla \phi_{p_2}(x, y, z, t) - i\rho_5 \mathbf{A}(z, t) \phi_{p_2}(x, y, z, t)|^2 \Big) \\
& \times |\phi_{A_2}(y, z, t)|^2 |\phi_{H_2}(z, t)|^2 dx dy dz dt.
\end{aligned} \tag{46}$$

Here, generically we have denoted

$$\nabla\phi(x, y, z, t) = (i\phi_t, \phi_{x_1}, \phi_{x_2}, \phi_{x_3}, \phi_{y_1}, \phi_{y_2}, \phi_{y_3}, \phi_{z_1}, \phi_{z_2}, \phi_{z_3})$$

where $i \in \mathbb{C}$ denotes the imaginary unit, so that

$$\nabla\phi \cdot \nabla\phi = -\phi_t^2 + \sum_{j=1}^3 (\phi_{x_j}^2 + \phi_{y_j}^2 + \phi_{z_j}^2).$$

$$\begin{aligned} E_{M_2} = & \frac{1}{2} \int_0^T \int_{\Omega} \int_{\Omega} \int_{\Omega} ((\gamma_7 |\nabla\phi_{p_3}(x, y, z, t) - i\rho_7 \mathbf{A}(z, t)\phi_{p_3}(x, y, z, t)|^2) \\ & \times |\phi_{A_3}(y, z, t)|^2 \frac{|\phi_{H_a^+}^2(z, t)|^2}{m_p}) dx dy dz dt \end{aligned} \quad (47)$$

and

$$\begin{aligned} E_{M_3} = & \int_0^T \int_{\Omega} \int_{\Omega} \int_{\Omega} ((\gamma_9 |\nabla\phi_{p_4}(x, y, z, t) - i\rho_9 \mathbf{A}(z, t)\phi_{p_4}(x, y, z, t)|^2) \\ & \times |\phi_{A_4}(y, z, t)|^2 \frac{|\phi_{H_b^+}^2(z, t)|^2}{m_p}) dx dy dz dt, \end{aligned} \quad (48)$$

$$E_{M_4} = \frac{\gamma_{11}}{2} \int_0^T \int_{\Omega} |\nabla\phi_{e_3}(z, t) - i\rho_{11} \mathbf{A}(z, t)\phi_{e_3}(z, t)|^2 dz dt,$$

and

$$E_{M_5} = \frac{\gamma_{12}}{2} \int_0^T \int_{\Omega} |\nabla\phi_{e_4}(z, t) - i\rho_{12} \mathbf{A}(z, t)\phi_{e_4}(z, t)|^2 dz dt.$$

Concerning the restrictions, considering the link between the two electrons, we define also the following functionals,

$$\begin{aligned} J_{Aux_1} = & \int_0^T \int_{\Omega} \int_{\Omega} E_1(y, z, t) \\ & \times \left(\int_{\Omega} (|\phi_{e_1}(x, y, z, t)|^2 + |\phi_{e_2}(x, y, z, t)|^2) dx - 2m_e \right) dy dz dt, \end{aligned} \quad (49)$$

$$J_{Aux_2} = \int_0^T \int_{\Omega} \int_{\Omega} E_2(y, z, t) \left(\int_{\Omega} |\phi_{p_1}(x, y, z, t)|^2 dx - m_p \right) dy dz dt, \quad (50)$$

$$J_{Aux_4} = \int_0^T \int_{\Omega} \int_{\Omega} E_5(y, z, t) \left(\int_{\Omega} |\phi_{p_2}(x, y, z, t)|^2 dx - m_p \right) dy dz dt, \quad (51)$$

$$J_{Aux_5} = \int_0^T \int_{\Omega} \int_{\Omega} E_7(y, z, t) \left(\int_{\Omega} |\phi_{p_3}(x, y, z, t)|^2 dx - m_p \right) dy dz dt, \quad (52)$$

$$J_{Aux_6} = \int_0^T \int_{\Omega} \int_{\Omega} E_9(y, z, t) \left(\int_{\Omega} |\phi_{p_4}(x, y, z, t)|^2 dx - m_p \right) dy dz dt, \quad (53)$$

$$J_{Aux_7} = \int_0^T \int_{\Omega} \int_{\Omega} E_{11}(z, t) \left(\int_{\Omega} |\phi_{A_1}(y, z, t)|^2 dy - 1 \right) dz dt, \quad (54)$$

$$J_{Aux_8} = \int_0^T \int_{\Omega} \int_{\Omega} E_{12}(z, t) \left(\int_{\Omega} |\phi_{A_2}(y, z, t)|^2 dy - 1 \right) dz dt, \quad (55)$$

$$J_{Aux_9} = \int_0^T \int_{\Omega} \int_{\Omega} E_{13}(z, t) \left(\int_{\Omega} |\phi_{A_3}(y, z, t)|^2 dy - 1 \right) dz dt, \quad (56)$$

$$J_{Aux_{10}} = \int_0^T \int_{\Omega} \int_{\Omega} E_{14}(z, t) \left(\int_{\Omega} |\phi_{A_4}(y, z, t)|^2 dy - 1 \right) dz dt, \quad (57)$$

$$\begin{aligned} J_{Aux_{11}} = & \int_0^T E_{15}(t) \left(\int_{\Omega} \rho_{H_2}(z, 0) dz \right. \\ & - \int_{\Omega} \rho_{H_2}(z, t) dz - \int_0^t \int_{\partial\Omega} \rho_{H_2}(z, \tau) \mathbf{v}_{H_2} \cdot \mathbf{n} dS d\tau \\ & - \int_{\Omega} \rho_{H_a^+}(z, t) dz - \int_0^t \int_{\partial\Omega} \rho_{H_a^+}(z, \tau) \mathbf{v}_{H_a^+} \cdot \mathbf{n} dS d\tau \\ & - \int_{\Omega} \rho_{H_b^+}(z, t) dz - \int_0^t \int_{\partial\Omega} \rho_{H_b^+}(z, \tau) \mathbf{v}_{H_b^+} \cdot \mathbf{n} dS d\tau \\ & - \int_{\Omega} \rho_{e_3}(z, t) dz - \int_0^t \int_{\partial\Omega} \rho_{e_3}(z, \tau) \mathbf{v}_{e_3} \cdot \mathbf{n} dS d\tau \\ & \left. - \int_{\Omega} \rho_{e_4}(z, t) dz - \int_0^t \int_{\partial\Omega} \rho_{e_4}(z, \tau) \mathbf{v}_{e_4} \cdot \mathbf{n} dS d\tau \right) dt \quad (58) \end{aligned}$$

We have also the following constraints

$$J_{Aux_{12}} = \int_0^T E_{16}(t) \left(\int_{\Omega} \rho_{e_3}(z, t) dz + \int_0^t \int_{\partial\Omega} \rho_{e_3}(z, \tau) \mathbf{v}_{e_3} \cdot \mathbf{n} dS d\tau - \int_{\Omega} \rho_{e_4}(z, t) dz - \int_0^t \int_{\partial\Omega} \rho_{e_4}(z, \tau) \mathbf{v}_{e_4} \cdot \mathbf{n} dS d\tau \right) dt \quad (59)$$

$$J_{Aux_{13}} = \int_0^T \int_{\Omega} E_{17}(x, t) \left(\mathbf{v}_{H_2} - \frac{\partial \mathbf{r}_{H_2}(x, t)}{\partial t} \right) dx dt,$$

$$J_{Aux_{14}} = \int_0^T \int_{\Omega} E_{18}(x, t) \left(\mathbf{v}_{H_a^+} - \frac{\partial \mathbf{r}_{H_a^+}(x, t)}{\partial t} \right) dx dt,$$

$$J_{Aux_{15}} = \int_0^T \int_{\Omega} E_{19}(x, t) \left(\mathbf{v}_{H_b^+} - \frac{\partial \mathbf{r}_{H_b^+}(x, t)}{\partial t} \right) dx dt,$$

$$J_{Aux_{16}} = \int_0^T \int_{\Omega} E_{20}(x, t) \left(\mathbf{v}_{e_1} - \frac{\partial \hat{\mathbf{r}}_{e_1}(x, t)}{\partial t} \right) dx dt,$$

$$J_{Aux_{17}} = \int_0^T \int_{\Omega} E_{21}(x, t) \left(\mathbf{v}_{p_1} - \frac{\partial \hat{\mathbf{r}}_{p_1}(x, t)}{\partial t} \right) dx dt,$$

$$J_{Aux_{18}} = \int_0^T \int_{\Omega} E_{23}(x, t) \left(\mathbf{v}_{e_2} - \frac{\partial \hat{\mathbf{r}}_{e_2}(x, t)}{\partial t} \right) dx dt,$$

$$J_{Aux_{19}} = \int_0^T \int_{\Omega} E_{24}(x, t) \left(\mathbf{v}_{p_1} - \frac{\partial \hat{\mathbf{r}}_{p_2}(x, t)}{\partial t} \right) dx dt,$$

$$J_{Aux_{20}} = \int_0^T \int_{\Omega} E_{26}(x, t) \left(\mathbf{v}_{p_3} - \frac{\partial \hat{\mathbf{r}}_{p_3}(x, t)}{\partial t} \right) dx dt,$$

$$J_{Aux_{22}} = \int_0^T \int_{\Omega} E_{28}(x, t) \left(\mathbf{v}_{p_4} - \frac{\partial \hat{\mathbf{r}}_{p_4}(x, t)}{\partial t} \right) dx dt,$$

$$J_{Aux_{23}} = \int_0^T \int_{\Omega} E_{30}(x, t) \left(\mathbf{v}_{e_3} - \frac{\partial \mathbf{r}_{e_3}(x, t)}{\partial t} \right) dx dt,$$

$$J_{Aux_{24}} = \int_0^T \int_{\Omega} E_{31}(x, t) \left(\mathbf{v}_{e_4} - \frac{\partial \mathbf{r}_{e_4}(x, t)}{\partial t} \right) dx dt,$$

$$J_{Aux_{25}} = \int_0^T \int_{\Omega} E_{32}(x, t) \left(\mathbf{v}_{A_1} - \frac{\partial \mathbf{r}_{A_1}(x, t)}{\partial t} \right) dx dt,$$

$$J_{Aux_{26}} = \int_0^T \int_{\Omega} E_{33}(x, t) \left(\mathbf{v}_{A_2} - \frac{\partial \mathbf{r}_{A_2}(x, t)}{\partial t} \right) dx dt,$$

$$J_{Aux_{27}} = \int_0^T \int_{\Omega} E_{34}(x, t) \left(\mathbf{v}_{A_3} - \frac{\partial \mathbf{r}_{A_3}(x, t)}{\partial t} \right) dx dt,$$

$$J_{Aux_{28}} = \int_0^T \int_{\Omega} E_{35}(x, t) \left(\mathbf{v}_{A_4} - \frac{\partial \mathbf{r}_{A_4}(x, t)}{\partial t} \right) dx dt,$$

Defining $\rho(z, t) = \rho_{H_2}(z, t) + \rho_{H_a^+}(z, t) + \rho_{H_b^+}(z, t) + \rho_{e_3}(z, t) + \rho_{e_4}(z, t)$, we define also

$$\begin{aligned} J_{Aux_{29}} = & - \int_0^T \int_{\Omega} \hat{P} \left(\frac{d\rho}{dt} + \rho_{H_2} \operatorname{div} \mathbf{v}_{H_2} + \rho_{H_a^+} \operatorname{div} \mathbf{v}_{H_a^+} \right. \\ & \left. + \rho_{H_b^+} \operatorname{div} \mathbf{v}_{H_b^+} + \rho_{e_3} \operatorname{div} \mathbf{v}_{e_3} + \rho_{e_4} \operatorname{div} \mathbf{v}_{e_4} \right) dz dt \quad (60) \end{aligned}$$

Moreover, considering the pressure and temperature scalar fields, we define

$$P = \frac{d(\hat{P}\rho)}{dt},$$

$$P_{H_2} = \frac{d(\hat{P}\rho_{H_2})}{dt},$$

$$P_{H_a^+} = \frac{d(\hat{P}\rho_{H_a^+})}{dt},$$

$$P_{H_b^+} = \frac{d(\hat{P}\rho_{H_b^+})}{dt},$$

$$P_{e_3} = \frac{d(\hat{P}\rho_{e_3})}{dt},$$

$$P_{e_4} = \frac{d(\hat{P}\rho_{e_4})}{dt},$$

$$\begin{aligned}
& (C_v)_{H_2} \rho_{H_2} T_{H_2} \\
= & \frac{1}{2} c \rho_{e_1}(z, t) \sqrt{c^2 - g_{jk}^{e_1} \frac{\partial(X_{H_2})_j}{\partial t} \frac{\partial(X_{H_2})_k}{\partial t}} \sqrt{-g^{e_1}} |\det X'_{H_2}| \\
& + \frac{1}{2} c \rho_{p_1}(z, t) \sqrt{c^2 - g_{jk}^{p_1} \frac{\partial(X_{H_2})_j}{\partial t} \frac{\partial(X_{H_2})_k}{\partial t}} \sqrt{-g^{p_1}} |\det X'_{H_2}| \\
& + \frac{1}{2} c \rho_{e_2}(z, t) \sqrt{c^2 - g_{jk}^{e_2} \frac{\partial(X_{H_2})_j}{\partial t} \frac{\partial(X_{H_2})_k}{\partial t}} \sqrt{-g^{e_2}} |\det X'_{H_2}| \\
& + \frac{1}{2} c \rho_{p_2}(z, t) \sqrt{c^2 - g_{jk}^{p_2} \frac{\partial(X_{H_2})_j}{\partial t} \frac{\partial(X_{H_2})_k}{\partial t}} \sqrt{-g^{p_2}} |\det X'_{H_2}| \quad (61)
\end{aligned}$$

$$\begin{aligned}
& (C_v)_{H_a^+} \rho_{H_a^+} T_{H_a^+} \\
= & \frac{1}{2} c \rho_{p_3}(z, t) \sqrt{c^2 - g_{jk}^{p_3} \frac{\partial(X_{H_a^+})_j}{\partial t} \frac{\partial(X_{H_a^+})_k}{\partial t}} \sqrt{-g^{p_3}} |\det X'_{H_a^+}| \quad (62)
\end{aligned}$$

$$\begin{aligned}
& (C_v)_{H_b^+} \rho_{H_b^+} T_{H_b^+} \\
= & \frac{1}{2} c \rho_{p_4}(z, t) \sqrt{c^2 - g_{jk}^{p_4} \frac{\partial(X_{H_b^+})_j}{\partial t} \frac{\partial(X_{H_b^+})_k}{\partial t}} \sqrt{-g^{p_4}} |\det X'_{H_b^+}| \quad (63)
\end{aligned}$$

and

$$\begin{aligned}
(C_v)_e \rho_e T_e &= \frac{1}{2} c \rho_{e_3}(z, t) \sqrt{c^2 - v_{e_3}^2} \sqrt{-g^{e_3}} \\
&+ \frac{1}{2} c \rho_{e_4}(z, t) \sqrt{c^2 - v_{e_4}^2} \sqrt{-g^{e_4}}. \quad (64)
\end{aligned}$$

Here we define the function space,

$$\begin{aligned}
V_{22} &= \left\{ \hat{T} = (T_{H_2}, T_{H_a^+}, T_{H_b^+}, T_e) \in W^{1,2}(\Omega \times [0, T]; \mathbb{R}^{1 \times 4}) \right. \\
&\quad \left. : \hat{T}(z, t) = T_0(z, t) \text{ on } \partial\Omega \times [0, T] \text{ and } \hat{T}(z, 0) = T_1(z) \text{ in } \Omega \right\}. \quad (65)
\end{aligned}$$

Moreover, we define the following entropy differentials

$$\begin{aligned}
dS_{H_2} &= -\hat{K}_{H_2} \frac{\rho_{H_2}}{\rho} \left(\ln \left(\frac{\rho_{H_2}}{e \rho} \right) - \omega_{H_2} \right) dx dt, \\
dS_{H_a^+} &= -\hat{K}_{H_a^+} \frac{\rho_{H_a^+}}{\rho} \left(\ln \left(\frac{\rho_{H_a^+}}{e \rho} \right) - \omega_{H_a^+} \right) dx dt,
\end{aligned}$$

$$\begin{aligned} dS_{H_b^+} &= -\hat{K}_{H_b^+} \frac{\rho_{H_b^+}}{\rho} \left(\ln \left(\frac{\rho_{H_b^+}}{e \rho} \right) - \omega_{H_b^+} \right) dxdt, \\ dS_{e_3} &= -\hat{K}_e \frac{\rho_{e_3}}{\rho} \left(\ln \left(\frac{\rho_{e_3}}{e \rho} \right) - \omega_{e_3} \right) dxdt, \\ dS_{e_4} &= -\hat{K}_e \frac{\rho_{e_4}}{\rho} \left(\ln \left(\frac{\rho_{e_4}}{e \rho} \right) - \omega_{e_4} \right) dxdt \end{aligned}$$

and the following functional

$$\begin{aligned} J_S &= \int_0^T \int_{\Omega} T_{H_2} dS_{H_2} + \int_0^T \int_{\Omega} T_{H_a^+} dS_{H_a^+} + \int_0^T \int_{\Omega} T_{H_b^+} dS_{H_b^+} \\ &\quad + \int_0^T \int_{\Omega} T_e dS_{e_3} + \int_0^T \int_{\Omega} T_e dS_{e_4}. \end{aligned} \quad (66)$$

We define also

$$\begin{aligned} S_{H_2} &= -\hat{K}_{H_2} \frac{\rho_{H_2}}{\rho} \left(\ln \left(\frac{\rho_{H_2}}{e \rho} \right) - \omega_{H_2} \right), \\ S_{H_a^+} &= -\hat{K}_{H_a^+} \frac{\rho_{H_a^+}}{\rho} \left(\ln \left(\frac{\rho_{H_a^+}}{e \rho} \right) - \omega_{H_a^+} \right), \\ S_{H_b^+} &= -\hat{K}_{H_b^+} \frac{\rho_{H_b^+}}{\rho} \left(\ln \left(\frac{\rho_{H_b^+}}{e \rho} \right) - \omega_{H_b^+} \right), \\ S_{e_3} &= -\hat{K}_e \frac{\rho_{e_3}}{\rho} \left(\ln \left(\frac{\rho_{e_3}}{e \rho} \right) - \omega_{e_3} \right), \\ S_{e_4} &= -\hat{K}_e \frac{\rho_{e_4}}{\rho} \left(\ln \left(\frac{\rho_{e_4}}{e \rho} \right) - \omega_{e_4} \right) \end{aligned}$$

and

$$E_S^M = T_{H_2} S_{H_2} + T_{H_a^+} S_{H_a^+} + T_{H_b^+} S_{H_b^+} + T_{H_e} (S_{e_3} + S_{e_4}).$$

With such results in mind, already including a term related to entropy, we define the restriction

$$\begin{aligned} &\rho_{H_2} (C_v)_{H_2} \frac{dT_{H_2}}{dt} + \rho_{H_a^+} (C_v)_{H_a^+} \frac{dT_{H_a^+}}{dt} + \rho_{H_b^+} (C_v)_{H_b^+} \frac{dT_{H_b^+}}{dt} + (C_v)_e \rho_e \frac{dT_e}{dt} \\ &= K_{H_2} \nabla^2 T_{H_2} + K_{H_a^+} \nabla^2 T_{H_a^+} + K_{H_b^+} \nabla^2 T_{H_b^+} + K_e \nabla^2 T_e \\ &\quad - P_{H_2} \operatorname{div} \mathbf{v}_{H_2} - P_{H_a^+} \operatorname{div} \mathbf{v}_{H_a^+} - P_{H_b^+} \operatorname{div} \mathbf{v}_{H_b^+} \\ &\quad - P_{e_3} \operatorname{div} \mathbf{v}_{e_3} - P_{e_4} \operatorname{div} \mathbf{v}_{e_4} + \frac{dE_S^M}{dt}. \end{aligned} \quad (67)$$

With such restrictions and definitions in mind, we define the following functionals,

$$\begin{aligned}
 J_{Aux_{30}} = & \int_0^T \int_{\Omega} E_{37}(z, t) \\
 & \times \left((C_v)_{H_2} \rho_{H_2} T_{H_2} - \frac{1}{2} c \rho_{e_1}(z, t) \sqrt{c^2 - g_{jk}^{e_1} \frac{\partial(X_{H_2})_j}{\partial t} \frac{\partial(X_{H_2})_k}{\partial t}} \sqrt{-g^{e_1}} |\det X'_{H_2}| \right. \\
 & - \frac{1}{2} c \rho_{p_1}(z, t) \sqrt{c^2 - g_{jk}^{p_1} \frac{\partial(X_{H_2})_j}{\partial t} \frac{\partial(X_{H_2})_k}{\partial t}} \sqrt{-g^{p_1}} |\det X'_{H_2}| \\
 & - \frac{1}{2} c \rho_{e_2}(z, t) \sqrt{c^2 - g_{jk}^{e_2} \frac{\partial(X_{H_2})_j}{\partial t} \frac{\partial(X_{H_2})_k}{\partial t}} \sqrt{-g^{e_2}} |\det X'_{H_2}| \\
 & \left. - \frac{1}{2} c \rho_{p_2}(z, t) \sqrt{c^2 - g_{jk}^{p_2} \frac{\partial(X_{H_2})_j}{\partial t} \frac{\partial(X_{H_2})_k}{\partial t}} \sqrt{-g^{p_2}} |\det X'_{H_2}| \right) dz dt \quad (68)
 \end{aligned}$$

$$\begin{aligned}
 J_{Aux_{31}} = & \int_0^T \int_{\Omega} E_{38}(z, t) \left((C_v)_{H_a^+} \rho_{H_a^+} T_{H_a^+} \right. \\
 & \left. - \frac{1}{2} c \rho_{p_3}(z, t) \sqrt{c^2 - g_{jk}^{p_3} \frac{\partial(X_{H_a^+})_j}{\partial t} \frac{\partial(X_{H_a^+})_k}{\partial t}} \sqrt{-g^{p_3}} |\det X'_{H_a^+}| \right) dz dt \quad (69)
 \end{aligned}$$

$$\begin{aligned}
 J_{Aux_{32}} = & \int_0^T \int_{\Omega} E_{39}(z, t) \left((C_v)_{H_b^+} \rho_{H_b^+} T_{H_b^+} \right. \\
 & \left. - \frac{1}{2} c \rho_{p_4}(z, t) \sqrt{c^2 - g_{jk}^{p_4} \frac{\partial(X_{H_b^+})_j}{\partial t} \frac{\partial(X_{H_b^+})_k}{\partial t}} \sqrt{-g^{p_4}} |\det X'_{H_b^+}| \right) dz dt \quad (70)
 \end{aligned}$$

and

$$\begin{aligned}
 J_{Aux_{33}} = & \int_0^T \int_{\Omega} E_{40}(z, t) \left((C_v)_e \rho_e T_e - \frac{1}{2} c \rho_{e_3}(z, t) \sqrt{c^2 - v_{e_3}^2} \sqrt{-g^{e_3}} \right. \\
 & \left. - \frac{1}{2} c \rho_{e_4}(z, t) \sqrt{c^2 - v_{e_4}^2} \sqrt{-g^{e_4}} \right) dz dt. \quad (71)
 \end{aligned}$$

With such results in mind, we define the restriction

$$\begin{aligned}
 J_{Aux34} = & \int_0^T \int_{\Omega} E_{41}(z, t) \\
 & \times \left(\rho_{H_2}(C_v)_{H_2} \frac{dT_{H_2}}{dt} + \rho_{H_a^+}(C_v)_{H_a^+} \frac{dT_{H_a^+}}{dt} + \rho_{H_b^+}(C_v)_{H_b^+} \frac{dT_{H_b^+}}{dt} + (C_v)_e \frac{dT_e}{dt} \right. \\
 & - K_{H_2} \nabla^2 T_{H_2} - K_{H_a^+} \nabla^2 T_{H_a^+} - K_{H_b^+} \nabla^2 T_{H_b^+} - K_e \rho_e \nabla^2 T_e \\
 & + P_{H_2} \operatorname{div} \mathbf{v}_{H_2} + P_{H_a^+} \operatorname{div} \mathbf{v}_{H_a^+} + P_{H_b^+} \operatorname{div} \mathbf{v}_{H_b^+} \\
 & \left. + P_{e_3} \operatorname{div} \mathbf{v}_{e_3} + P_{e_4} \operatorname{div} \mathbf{v}_{e_4} - \frac{dE_S^M}{dt} \right) dz dt
 \end{aligned} \tag{72}$$

Finally, we define the following functionals,

$$\begin{aligned}
 J_{Aux35} = & \int_0^T \int_{\Omega} \int_{\Omega} E_{50}(z, t) (\rho_{H_2}(z, t) \\
 & - \int_{\Omega} \int_{\Omega} (|\phi_{e_1}(x, y, z, t)|^2 + |\phi_{p_1}(x, y, z, t)|^2) \\
 & \times \frac{|\phi_{A_1}(y, z, t)|^2}{2m_e + 2m_p} |\phi_{H_2}(z, t)|^2 \\
 & - (|\phi_{e_2}(x, y, z, t)|^2 + |\phi_{p_2}(x, y, z, t)|^2) \\
 & \times \frac{|\phi_{A_2}(y, z, t)|^2}{2m_e + 2m_p} |\phi_{H_2}(z, t)|^2) dx dy dz dt,
 \end{aligned} \tag{73}$$

$$\begin{aligned}
 J_{Aux36} = & \int_0^T \int_{\Omega} \int_{\Omega} E_{60}(z, t) \left(\rho_{H_a^+}(z, t) \right. \\
 & - \int_{\Omega} \int_{\Omega} \left(\frac{|\phi_{p_3}(x, y, z, t)|^2}{m_p} \right) \\
 & \times |\phi_{A_3}(y, z, t)|^2 |\phi_{H_a^+}(z, t)|^2) dx dy dz dt,
 \end{aligned} \tag{74}$$

$$\begin{aligned}
& J_{Au x_{37}} \\
&= \int_0^T \int_{\Omega} \int_{\Omega} E_{70}(z, t) \left(\rho_{H_b^+}(z, t) \right. \\
&\quad \left. - \int_{\Omega} \int_{\Omega} \left(\frac{|\phi_{p_4}(x, y, z, t)|^2}{m_p} \right) \right. \\
&\quad \left. \times |\phi_{A_4}(y, z, t)|^2 |\phi_{H_b^+}(z, t)|^2 \right) dx dy dz dt, \tag{75}
\end{aligned}$$

6 The main functional

Here we define

$$(\mathbf{A}, V) \in V_{23} = W^{1,2}(\Omega \times [0, T]; \mathbb{R}^3) \times W^{1,2}(\Omega \times [0, T]),$$

where $\mathbf{A}$ is a magnetic potential and V is an electric potential.

Moreover, we denote by ρ^e , m_e an electron charge and mass and ρ^p , m_p a proton charge and mass, respectively. Moreover, we define

$$K_1 = K_0 \frac{\rho_e}{m_e}$$

and $K_2 = K_0 \frac{\rho^p}{m_p}$, for an appropriate real constant $K_0 > 0$, and define the functionals

$$J : V_1 \times \cdots \times V_{23} \rightarrow \mathbb{R}$$

and

$$J_1 : V_1 \times \cdots \times V_{23} \rightarrow \mathbb{R},$$

by

$$\begin{aligned}
J = & \frac{1}{2} \int_0^T \int_{\Omega} \rho_{H_2} \mathbf{v}_{H_2} \cdot \mathbf{v}_{H_2} \, dz \, dt + \int_0^T \int_{\Omega} \frac{\rho_{e_1}}{\sqrt{1 - \frac{v_{e_1}^2}{c^2}}} \mathbf{v}_{e_1} \cdot \mathbf{v}_{H_2} \, dz \, dt \\
& + \int_0^T \int_{\Omega} \frac{\rho_{p_1}}{\sqrt{1 - \frac{v_{p_1}^2}{c^2}}} \mathbf{v}_{p_1} \cdot \mathbf{v}_{H_2} \, dz \, dt + \int_0^T \int_{\Omega} \frac{\rho_{e_2}}{\sqrt{1 - \frac{v_{e_2}^2}{c^2}}} \mathbf{v}_{e_2} \cdot \mathbf{v}_{H_2} \, dz \, dt \\
& + \int_0^T \int_{\Omega} \frac{\rho_{p_2}}{\sqrt{1 - \frac{v_{p_2}^2}{c^2}}} \mathbf{v}_{p_2} \cdot \mathbf{v}_{H_2} \, dz \, dt \\
& + \frac{1}{2} \int_0^T \int_{\Omega} \rho_{H_a^+} \mathbf{v}_{H_a^+} \cdot \mathbf{v}_{H_a^+} \, dz \, dt \\
& + \int_0^T \int_{\Omega} \frac{\rho_{p_3}}{\sqrt{1 - \frac{v_{p_3}^2}{c^2}}} \mathbf{v}_{p_3} \cdot \mathbf{v}_{H_a^+} \, dz \, dt \\
& + \frac{1}{2} \int_0^T \int_{\Omega} \rho_{H_b^+} \mathbf{v}_{H_b^+} \cdot \mathbf{v}_{H_b^+} \, dz \, dt \\
& + \int_0^T \int_{\Omega} \frac{\rho_{p_4}}{\sqrt{1 - \frac{v_{p_4}^2}{c^2}}} \mathbf{v}_{p_4} \cdot \mathbf{v}_{H_b^+} \, dz \, dt \\
& - K_1 \int_0^T \int_{\Omega} \int_{\Omega} \int_{\Omega} \hat{\rho}_{e_1} \mathbf{v}_{e_1} \cdot \mathbf{A} \, dx \, dy \, dz \, dt \\
& - K_2 \int_0^T \int_{\Omega} \int_{\Omega} \int_{\Omega} \hat{\rho}_{p_1} \mathbf{v}_{p_1} \cdot \mathbf{A} \, dx \, dy \, dz \, dt \\
& - K_1 \int_0^T \int_{\Omega} \int_{\Omega} \int_{\Omega} \hat{\rho}_{e_2} \mathbf{v}_{e_2} \cdot \mathbf{A} \, dx \, dy \, dz \, dt \\
& - K_2 \int_0^T \int_{\Omega} \int_{\Omega} \int_{\Omega} \hat{\rho}_{p_2} \mathbf{v}_{p_2} \cdot \mathbf{A} \, dx \, dy \, dz \, dt \\
& - K_2 \int_0^T \int_{\Omega} \int_{\Omega} \int_{\Omega} \hat{\rho}_{p_3} \mathbf{v}_{p_3} \cdot \mathbf{A} \, dx \, dy \, dz \, dt \\
& - K_2 \int_0^T \int_{\Omega} \int_{\Omega} \int_{\Omega} \hat{\rho}_{p_4} \mathbf{v}_{p_4} \cdot \mathbf{A} \, dx \, dy \, dz \, dt \\
& - K_1 \int_0^T \int_{\Omega} \rho_{e_3} \mathbf{v}_{e_3} \cdot \mathbf{A} \, dz \, dt \\
& - K_1 \int_0^T \int_{\Omega} \rho_{e_4} \mathbf{v}_{e_4} \cdot \mathbf{A} \, dz \, dt \\
& - \mathbf{g} \cdot \rho_{H_2} \mathbf{r}_{H_2} - \mathbf{g} \cdot \rho_{H_a^+} \mathbf{r}_{H_a^+} - \mathbf{g} \cdot \rho_{H_b^+} \mathbf{r}_{H_b^+} \\
& - \mathbf{g} \cdot \rho_{e_3} \mathbf{r}_{e_3} - \mathbf{g} \cdot \rho_{e_4} \mathbf{r}_{e_4}.
\end{aligned} \tag{76}$$

and, generically denoting

$$\hat{V}(\mathbf{r}_{H_a^+}, \mathbf{r}_{H_b^+}, \mathbf{r}_{e_3}, \mathbf{r}_{e_4}) = V(z, t)$$

and

$$\mathbf{B} = \text{Curl } \mathbf{A} - \mathbf{B}_0,$$

we also define

$$\begin{aligned} J_1 = & - \int_0^T \int_{\Omega} \int_{\Omega} \int_{\Omega} V(z, t) \\ & \times (K_1 \hat{\rho}_{e_1} + K_2 \hat{\rho}_{p_1} + K_1 \hat{\rho}_{e_2} + K_2 \hat{\rho}_{p_2} \\ & + K_2 \hat{\rho}_{p_3} + K_2 \hat{\rho}_{p_4} + K_1 \hat{\rho}_{e_3} + K_1 \hat{\rho}_{e_4}) \, dx \, dy \, dz \, dt \\ & + \frac{1}{8\pi} \|\text{Curl } \mathbf{A}(z, t) - \mathbf{B}_0\|_{0,2}^2 \\ & - \frac{1}{8\pi} \left\| \nabla_z V(z, t) + \frac{1}{c} \frac{\partial \mathbf{A}(z, t)}{\partial t} \right\|_{0,2}^2 \\ & - K_2 \int_0^T \int_{\Omega} |\phi_{H_a^+}|^2 \mathbf{B}(x, t) \times \frac{\partial \mathbf{r}_{H_a^+}(x, t)}{\partial t} \cdot (\mathbf{r}_{H_a^+}(\varepsilon t, x) - (\mathbf{r}_0)_{H_a^+}(x)) \, dx dt \\ & - K_2 \int_0^T \int_{\Omega} |\phi_{H_b^+}|^2 \mathbf{B}(x, t) \times \frac{\partial \mathbf{r}_{H_b^+}(x, t)}{\partial t} \cdot (\mathbf{r}_{H_b^+}(\varepsilon t, x) - (\mathbf{r}_0)_{H_b^+}(x)) \, dx dt \\ & - K_1 \int_0^T \int_{\Omega} |\phi_{e_3}|^2 \mathbf{B}(x, t) \times \frac{\partial \mathbf{r}_{e_3}(x, t)}{\partial t} \cdot (\mathbf{r}_{e_3}(\varepsilon t, x) - (\mathbf{r}_0)_{e_3}(x)) \, dx dt \\ & - K_1 \int_0^T \int_{\Omega} |\phi_{e_4}|^2 \mathbf{B}(x, t) \times \frac{\partial \mathbf{r}_{e_4}(x, t)}{\partial t} \cdot (\mathbf{r}_{e_4}(\varepsilon t, x) - (\mathbf{r}_0)_{e_4}(x)) \, dx dt \quad (77) \end{aligned}$$

where

$$\mathbf{B} = \mathbf{B}_0 - \text{Curl } \mathbf{A}$$

is the total magnetic field, $\mathbf{B}_0$ is an external magnetic field, $\mathbf{A} = (A_1, A_2, A_3)$ is the magnetic potential,

$$\hat{V}(\mathbf{r}_{H_a^+}, \mathbf{r}_{H_b^+}, \mathbf{r}_{e_3}, \mathbf{r}_{e_4}) = V(z, t)$$

is the electric potential and

$$\mathbf{E} = \nabla V(z, t) + \frac{1}{c} \frac{\partial \mathbf{A}}{\partial t},$$

is the electric field.

The variation of $J + J_1$ in $\mathbf{r}_{H_a^+}$ which lead us to the correct Euler-Lagrange equation is defined by

$$\begin{aligned} & \hat{\delta}(J_1)_{\mathbf{r}_{H_a^+}}(\mathbf{r}_{H_a^+}, \mathbf{r}_{H_a^+}(\varepsilon t, x), \cdot, \phi_{H_a^+}, \phi_{H_b^+}, \phi_{e_3}, \phi_{e_4}, \mathbf{A}, V; \varphi) = \\ & \lim_{h \rightarrow 0} \left[J_1(\mathbf{r}_{H_a^+} + h\varphi, \mathbf{r}_{H_a^+}(\varepsilon t, x) + h\varphi, \cdot, \phi_{H_a^+}, \phi_{H_b^+}, \phi_{e_3}, \phi_{e_4}, \mathbf{A}, V) \right. \\ & \quad \left. - J_1(\mathbf{r}_{H_a^+}, \mathbf{r}_{H_a^+}(\varepsilon t, x), \cdot, \phi_{H_a^+}, \phi_{H_b^+}, \phi_{e_3}, \phi_{e_4}, \mathbf{A}, V) \right] / h, \\ & \forall \varphi \in C_c^\infty(\Omega \times [0, T]; \mathbb{R}^3). \end{aligned} \quad (78)$$

The corresponding Euler-Lagrange equation stands for

$$\begin{aligned} & \frac{\partial}{\partial t} \left(|\phi_{H_a^+}|^2 \frac{\partial \mathbf{r}_{H_a^+}(x, t)}{\partial t} \right) - K_2 \frac{\partial}{\partial t} (|\phi_{H_a^+}|^2 \mathbf{A}) \\ & \frac{\partial \hat{V}}{\partial \mathbf{r}_{H_a^+}} (K_2 |\phi_{H_a^+}|^2 + K_2 |\phi_{H_b^+}|^2 + K_1 |\phi_{e_3}|^2 + K_1 |\phi_{e_4}|^2) \\ & + K_2 |\phi_{H_a^+}|^2 \mathbf{B} \times \frac{\partial \mathbf{r}_{H_a^+}}{\partial t} + \mathcal{O}(\varepsilon) \\ & - \frac{1}{4\pi} \operatorname{div} \mathbf{E} \frac{\partial \hat{V}}{\partial \mathbf{r}_{H_a^+}} = 0. \end{aligned} \quad (79)$$

Considering a Maxwell equation in question and letting $\varepsilon \rightarrow 0$, we obtain

$$\begin{aligned} & \frac{\partial}{\partial t} \left(|\phi_{H_a^+}|^2 \frac{\partial \mathbf{r}_{H_a^+}(x, t)}{\partial t} \right) - K_2 \frac{\partial}{\partial t} (|\phi_{H_a^+}|^2 \mathbf{A}) \\ & + K_2 |\phi_{H_a^+}|^2 \mathbf{B} \times \frac{\partial \mathbf{r}_{H_a^+}}{\partial t} = 0. \end{aligned} \quad (80)$$

We highlight the solution of the concerned system including such an Euler-Lagrange equation is computable, through the Newton's method for example, by expanding $J + J_1$ as a quadratic approximate function in φ about $(\mathbf{r}, \mathbf{r}(\varepsilon t, x))$ in each iteration.

Remark 6.1. The variation of $J + J_1$ in $\mathbf{A}$ stands for

$$\begin{aligned} & \operatorname{curl} (\operatorname{curl} \mathbf{A} - \mathbf{B}_0) + \frac{1}{c} \frac{\partial}{\partial t} \left(\nabla \hat{V}(\mathbf{r}_{H_a^+}, \mathbf{r}_{H_b^+}, \mathbf{r}_{e_3}, \mathbf{r}_{e_4}) + \frac{1}{c} \frac{\partial \mathbf{A}}{\partial t} \right) \\ & + \mathcal{O}(\varepsilon) + 4\pi K_2 |\phi_{H_a^+}|^2 \frac{\partial \mathbf{r}_{H_a^+}}{\partial t} + 4\pi K_2 |\phi_{H_b^+}|^2 \frac{\partial \mathbf{r}_{H_b^+}}{\partial t} \\ & + 4\pi K_1 |\phi_{e_3}|^2 \frac{\partial \mathbf{r}_{e_3}}{\partial t} + 4\pi K_1 |\phi_{e_4}|^2 \frac{\partial \mathbf{r}_{e_4}}{\partial t} \\ & = 0. \end{aligned} \quad (81)$$

Letting $\varepsilon \rightarrow 0$, we have the following Maxwell equation

$$\text{curl } \mathbf{B} - \frac{1}{c} \frac{\partial \mathbf{E}}{\partial t} - 4\pi \tilde{\mathbf{J}} = \mathbf{0},$$

where

$$\begin{aligned} \tilde{\mathbf{J}} = & K_2 |\phi_{H_a^+}|^2 \frac{\partial \mathbf{r}_{H_a^+}}{\partial t} + K_2 |\phi_{H_b^+}|^2 \frac{\partial \mathbf{r}_{H_b^+}}{\partial t} \\ & + K_1 |\phi_{e_3}|^2 \frac{\partial \mathbf{r}_{e_3}}{\partial t} + K_1 |\phi_{e_4}|^2 \frac{\partial \mathbf{r}_{e_4}}{\partial t}. \end{aligned} \quad (82)$$

The variation of $J + J_1$ in V stands for

$$\begin{aligned} & -4\pi K_2 (|\phi_{H_a^+}|^2 + |\phi_{H_b^+}|^2) - 4\pi K_1 (|\phi_{e_3}|^2 + |\phi_{e_4}|^2) \\ & + \text{div} \left(\nabla \hat{V}(\mathbf{r}_{H_a^+}, \mathbf{r}_{H_b^+}, \mathbf{r}_{e_3}, \mathbf{r}_{e_4}) + \frac{1}{c} \frac{\partial \mathbf{A}}{\partial t} \right) = \mathbf{0}, \end{aligned} \quad (83)$$

so that we obtain another Maxwell equation

$$\text{div } \mathbf{E} = 4\pi K_2 (|\phi_{H_a^+}|^2 + |\phi_{H_b^+}|^2) + 4\pi K_1 (|\phi_{e_3}|^2 + |\phi_{e_4}|^2)$$

Moreover, from

$$\mathbf{B} = - \text{curl } \mathbf{A} + \mathbf{B}_0$$

and assuming $\text{div } (\mathbf{B}_0) = 0$, we have got

$$\text{div } \mathbf{B} = - \text{div } (\text{curl } \mathbf{A}) = 0,$$

which is a third Maxwell equation.

Finally, the fourth Maxwell equation is obtained recalling that

$$\mathbf{E} = \nabla \hat{V}(\mathbf{r}_{H_a^+}, \mathbf{r}_{H_b^+}, \mathbf{r}_{e_3}, \mathbf{r}_{e_4}) + \frac{1}{c} \frac{\partial \mathbf{A}}{\partial t},$$

so that

$$\text{curl } \mathbf{E} = \text{curl } (\nabla V) + \frac{1}{c} \text{curl} \left(\frac{\partial \mathbf{A}}{\partial t} \right),$$

and therefore,

$$\text{curl } \mathbf{E} - \frac{1}{c} \left(\frac{\partial \text{curl } \mathbf{A}}{\partial t} \right) = \mathbf{0},$$

that is,

$$\text{curl } \mathbf{E} - \frac{1}{c} \left(\frac{\partial (-\mathbf{B} + \mathbf{B}_0)}{\partial t} \right) = \mathbf{0}.$$

Thus, if $\mathbf{B}_0$ is time independent, that is,

$$\frac{\partial \mathbf{B}_0}{\partial t} = \mathbf{0},$$

we have

$$\text{curl } \mathbf{E} + \frac{1}{c} \left(\frac{\partial \mathbf{B}}{\partial t} \right) = \mathbf{0}.$$

In summary, we have got all the four Maxwell equations as necessary conditions for a extremal point of J_3 .

The final variational formulation J_{total} for such an ionization process stands for

$$\begin{aligned} J_{total} = & J + J_1 - J_S \\ & - \sum_{k=1}^8 E_{C_k} + E_{in} \\ & + \sum_{k=1}^5 E_{M_k} + \sum_{k=1}^{37} J_{Aux_k}. \end{aligned} \quad (84)$$

Observe that the extremal equation

$$\frac{\partial J_{total}}{\partial \rho_{H_2}} = \mathbf{0}$$

stands for

$$\begin{aligned} & \frac{\partial J}{\partial \rho_{H_2}} - \frac{\partial J_S}{\partial \rho_{H_2}} + \frac{\partial E_{in}}{\partial \rho_{H_2}} + \frac{\partial J_{Aux_{30}}}{\partial \rho_{H_2}} + \frac{\partial J_{Aux_{11}}}{\partial \rho_{H_2}} \\ & + \frac{\partial J_{Aux_{34}}}{\partial \rho_{H_2}} + \frac{d\hat{P}}{dt} - \hat{P} \operatorname{div} \mathbf{v}_{H_2} + E_{50}(z, t) \\ = & \mathbf{0}, \end{aligned} \quad (85)$$

where,

$$\frac{\partial J}{\partial \rho_{H_2}} = \frac{1}{2} \mathbf{v}_{H_2} \cdot \mathbf{v}_{H_2} - \mathbf{g} \cdot \mathbf{r}_{H_2}.$$

Furthermore,

$$\frac{\partial E_{in}}{\partial \rho_{H_2}} = \alpha_1 \rho_{H_2} - \beta_1 \quad (86)$$

$$\begin{aligned}\frac{\partial J_{Aux30}}{\partial \rho_{H_2}} &= E_{37}(z, t) C_{v_{H_2}} T_{H_2}, \\ \frac{\partial J_{Aux34}}{\partial \rho_{H_2}} &= -E_{41}(z, t) \mathbf{g} \cdot \mathbf{v}_{H_2} + E_{41}(z, t) \frac{dE_S^M}{dt}.\end{aligned}$$

and $\frac{\partial J_{Aux11}}{\partial \rho_{H_2}}$ is a Gâteaux differential related to the following variation,

$$\begin{aligned}& \delta J_{Aux11}(\rho_{H_2}; \varphi) \\ &= \int_0^T E_{15}(t) \left(\int_{\Omega} \varphi(y, 0) dy - \int_{\Omega} \varphi(y, t) dy \right. \\ & \quad \left. - \int_0^t \int_{\Omega} \varphi(y, \tau) \mathbf{v}_{H_2} \cdot \mathbf{n} dS d\tau \right) dt,\end{aligned}\tag{87}$$

$\forall \varphi \in C^\infty(\Omega \times [0, T])$.

Observe also that

$$P_{H_2} = \frac{d(\hat{P}\rho_{H_2})}{dt},$$

so that

$$P_{H_2} = \frac{d\hat{P}}{dt} \rho_{H_2} + \hat{P} \frac{d\rho_{H_2}}{dt}.$$

Thus,

$$\frac{d\hat{P}}{dt} = \frac{P_{H_2}}{\rho_{H_2}} - \frac{\hat{P}}{\rho_{H_2}} \frac{d\rho_{H_2}}{dt}.$$

From such last results, we may infer that

$$\begin{aligned}& \frac{\partial J}{\partial \rho_{H_2}} - \frac{\partial J_S}{\partial \rho_{H_2}} + \frac{\partial E_{in}}{\partial \rho_{H_2}} + \frac{\partial J_{Aux30}}{\partial \rho_{H_2}} + \frac{\partial J_{Aux11}}{\partial \rho_{H_2}} \\ & + \frac{\partial J_{Aux34}}{\partial \rho_{H_2}} + \frac{d\hat{P}}{dt} - \hat{P} \operatorname{div} \mathbf{v}_{H_2} + E_{50}(z, t) \\ &= \frac{\partial J}{\partial \rho_{H_2}} - \frac{\partial J_S}{\partial \rho_{H_2}} + \frac{\partial E_{in}}{\partial \rho_{H_2}} + \frac{\partial J_{Aux30}}{\partial \rho_{H_2}} + \frac{\partial J_{Aux34}}{\partial \rho_{H_2}} + \frac{\partial J_{Aux11}}{\partial \rho_{H_2}} \\ & \quad \frac{P_{H_2}}{\rho_{H_2}} - \frac{\hat{P}}{\rho_{H_2}} \frac{d\rho_{H_2}}{dt} - \hat{P} \operatorname{div} \mathbf{v}_{H_2} + E_{50}(z, t) \\ &= \frac{\partial J}{\partial \rho_{H_2}} - \frac{\partial J_S}{\partial \rho_{H_2}} + \frac{\partial E_{in}}{\partial \rho_{H_2}} + \frac{\partial J_{Aux30}}{\partial \rho_{H_2}} \\ & \quad + \frac{\partial J_{Aux34}}{\partial \rho_{H_2}} + \frac{\partial J_{Aux11}}{\partial \rho_{H_2}} + \frac{P_{H_2}}{\rho_{H_2}} + E_{50}(z, t) \\ &= \mathbf{0}.\end{aligned}\tag{88}$$

Moreover, from the extremal equation

$$\frac{\partial J_{total}}{\partial \phi_{e_1}} = 0,$$

we obtain

$$\begin{aligned} & -\frac{\partial \hat{\rho}_{e_1}}{\partial \phi_{e_1}} c \sqrt{c^2 - g_{jk}^{e_1} \frac{\partial (X_{H_2})_j}{\partial t} \frac{\partial (X_{H_2})_k}{\partial t}} \sqrt{-g^{e_1}} |\det X'_{H_2}| \\ & + \frac{\partial \hat{\rho}_{e_1}}{\partial \phi_{e_1}} \mathbf{v}_{e_1} \cdot \mathbf{v}_{H_2} / \sqrt{1 - \frac{v_{e_1}^2}{c^2}} \\ & - \frac{\partial \hat{\rho}_{e_1}}{\partial \phi_{e_1}} \mathbf{v}_{e_1} \cdot \mathbf{A} + K_1 V(z, t) \frac{\partial \hat{\rho}_{e_1}}{\partial \phi_{e_1}} \\ & + 2E_1(y, z, t) \phi_{e_1} + \frac{\partial E_{in}}{\partial \rho_{e_1}} \frac{\partial \hat{\rho}_{e_1}}{\partial \phi_{e_1}} \\ & - E_{50}(z, t) \frac{\phi_{e_1}(x, y, z, t)}{2m_e + 2m_p} |A_1(y, z, t)|^2 |\phi_{H_2}(z, t)|^2 \\ & = 0, \end{aligned} \tag{89}$$

where

$$\frac{\partial \hat{\rho}_{e_1}}{\partial \phi_{e_1}} = \frac{\phi_{e_1}}{m_e} |\phi_{A_1}|^2 \rho_{H_2},$$

and

$$\begin{aligned} & \frac{\partial E_{in}}{\partial \rho_{e_1}} \frac{\partial \hat{\rho}_{e_1}}{\partial \phi_{e_1}} \\ & = 2\alpha_1 \rho_{H_2} \left(\frac{|\phi_{e_1}(x, y, z, t)|}{2m_e + m_p} \right) |\phi_{A_1}(y, z, t)|^2 \rho_{H_2} \\ & - \beta_1 \left(\frac{\phi_{e_1}(x, y, z, t)}{2m_e + 2m_p} \right) |\phi_{A_1}(y, z, t)|^2 \rho_{H_2}. \end{aligned} \tag{90}$$

Denoting

$$E_{50}(z, t) = -\frac{P_{H_2}}{\rho_{H_2}} - B,$$

where

$$B = \frac{\partial J}{\partial \rho_{H_2}} - \frac{\partial J_S}{\partial \rho_{H_2}} + \frac{\partial E_{in}}{\partial \rho_{H_2}} + \frac{\partial J_{Aux_{30}}}{\partial \rho_{H_2}} + \frac{\partial J_{Aux_{34}}}{\partial \rho_{H_2}} + \frac{\partial J_{Aux_{11}}}{\partial \rho_{H_2}},$$

from the last previous equation, we obtain,

$$\begin{aligned}
& -\frac{\partial \hat{\rho}_{e_1}}{\partial \phi_{e_1}} c \sqrt{c^2 - g_{jk}^{e_1} \frac{\partial (X_{H_2})_j}{\partial t} \frac{\partial (X_{H_2})_k}{\partial t}} \sqrt{-g^{e_1}} |\det X'_{H_2}| \\
& + \frac{\partial \hat{\rho}_{e_1}}{\partial \phi_{e_1}} \mathbf{v}_{e_1} \cdot \mathbf{v}_{H_2} / \sqrt{1 - \frac{v_{e_1}^2}{c^2}} \\
& - \frac{\partial \hat{\rho}_{e_1}}{\partial \phi_{e_1}} \mathbf{v}_{e_1} \cdot \mathbf{A} + K_1 V(x, y, z, t) \frac{\partial \hat{\rho}_{e_1}}{\partial \phi_{e_1}} \\
& + 2E_1(y, z, t) \phi_{e_1} + \frac{\partial E_{in}}{\partial \rho_{e_1}} \frac{\partial \hat{\rho}_{e_1}}{\partial \phi_{e_1}} \\
& + \left(\frac{P_{H_2}}{\rho_{H_2}} + B \right) \frac{\phi_{e_1}(x, y, z, t)}{2m_e + 2m_p} |A_1(y, z, t)|^2 |\phi_{H_2}(z, t)|^2 \\
& = 0.
\end{aligned} \tag{91}$$

Multiplying both sides of this last equation by $\phi_{e_1}^*$, we have

$$\begin{aligned}
& -\hat{\rho}_{e_1} c \sqrt{c^2 - g_{jk}^{e_1} \frac{\partial (X_{H_2})_j}{\partial t} \frac{\partial (X_{H_2})_k}{\partial t}} \sqrt{-g^{e_1}} |\det X'_{H_2}| \\
& + \hat{\rho}_{e_1} \mathbf{v}_{e_1} \cdot \mathbf{v}_{H_2} / \sqrt{1 - \frac{v_{e_1}^2}{c^2}} \\
& - \hat{\rho}_{e_1} \mathbf{v}_{e_1} \cdot \mathbf{A} + K_1 V(z, t) \hat{\rho}_{e_1} \\
& + 2E_1(y, z, t) |\phi_{e_1}|^2 + \frac{\partial E_{in}}{\partial \rho_{e_1}} \hat{\rho}_{e_1} \\
& + \left(\frac{P_{H_2}}{\rho_{H_2}} + B \right) \frac{2|\phi_{e_1}(x, y, z, t)|^2}{2m_e + 2m_p} |A_1(y, z, t)|^2 |\phi_{H_2}(z, t)|^2 \\
& = 0.
\end{aligned} \tag{92}$$

Similarly, we may obtain

$$\begin{aligned}
& -\hat{\rho}_{p_1} c \sqrt{c^2 - g_{jk}^{p_1} \frac{\partial (X_{H_2})_j}{\partial t} \frac{\partial (X_{H_2})_k}{\partial t}} \sqrt{-g^{p_1}} |\det X'_{H_2}| \\
& + \hat{\rho}_{p_1} \mathbf{v}_{p_1} \cdot \mathbf{v}_{H_2} / \sqrt{1 - \frac{v_{p_1}^2}{c^2}} \\
& - \hat{\rho}_{p_1} \mathbf{v}_{p_1} \cdot \mathbf{A} + K_1 V(z, t) \hat{\rho}_{p_1} \\
& + E_5(y, z, t) |\phi_{p_1}|^2 + \frac{\partial E_{in}}{\partial \rho_{p_1}} \hat{\rho}_{p_1} \\
& + \left(\frac{P_{H_2}}{\rho_{H_2}} + B \right) \frac{2|\phi_{p_1}(x, y, z, t)|^2}{2m_e + 2m_p} |A_1(y, z, t)|^2 |\phi_{H_2}(z, t)|^2 \\
& = 0,
\end{aligned} \tag{93}$$

$$\begin{aligned}
& -\hat{\rho}_{e_2} c \sqrt{c^2 - g_{jk}^{e_2} \frac{\partial(X_{H_2})_j}{\partial t} \frac{\partial(X_{H_2})_k}{\partial t}} \sqrt{-g^{e_2}} |\det X'_{H_2}| \\
& + \hat{\rho}_{e_2} \mathbf{v}_{e_2} \cdot \mathbf{v}_{H_2} / \sqrt{1 - \frac{v_{e_2}^2}{c^2}} \\
& - \hat{\rho}_{e_2} \mathbf{v}_{e_2} \cdot \mathbf{A} + K_1 V(z, t) \hat{\rho}_{e_2} \\
& + 2E_1(y, z, t) |\phi_{e_2}|^2 + \frac{\partial E_{in}}{\partial \rho_{e_2}} \hat{\rho}_{e_2} \\
& + \left(\frac{P_{H_2}}{\rho_{H_2}} + B \right) \frac{2|\phi_{e_2}(x, y, z, t)|^2}{2m_e + 2m_p} |A_2(y, z, t)|^2 |\phi_{H_2}(z, t)|^2 \\
& = 0
\end{aligned} \tag{94}$$

and

$$\begin{aligned}
& -\hat{\rho}_{p_2} c \sqrt{c^2 - g_{jk}^{p_2} \frac{\partial(X_{H_2})_j}{\partial t} \frac{\partial(X_{H_2})_k}{\partial t}} \sqrt{-g^{p_2}} |\det X'_{H_2}| \\
& + \hat{\rho}_{p_2} \mathbf{v}_{p_2} \cdot \mathbf{v}_{H_2} / \sqrt{1 - \frac{v_{p_2}^2}{c^2}} \\
& - \hat{\rho}_{p_2} \mathbf{v}_{p_2} \cdot \mathbf{A} + K_1 V(z, t) \hat{\rho}_{p_2} \\
& + E_7(y, z, t) |\phi_{p_2}|^2 + \frac{\partial E_{in}}{\partial \rho_{p_2}} \hat{\rho}_{p_2} \\
& + \left(\frac{P_{H_2}}{\rho_{H_2}} + B \right) \frac{2|\phi_{p_2}(x, y, z, t)|^2}{2m_e + 2m_p} |A_2(y, z, t)|^2 |\phi_{H_2}(z, t)|^2 \\
& = 0.
\end{aligned} \tag{95}$$

where

$$\begin{aligned}
& \frac{\partial E_{in}}{\partial \rho_{e_2}} \frac{\partial \hat{\rho}_{e_2}}{\partial \phi_{e_2}} \\
& = 2\alpha_1 \rho_{H_2} \left(\frac{|\phi_{e_2}(x, y, z, t)|}{2m_e + 2m_p} \right) |\phi_{A_2}(y, z, t)|^2 \rho_{H_2} \\
& - \beta_1 \left(\frac{\phi_{e_2}(x, y, z, t)}{2m_e + 2m_p} \right) |\phi_{A_2}(y, z, t)|^2 \rho_{H_2},
\end{aligned} \tag{96}$$

$$\begin{aligned}
& \frac{\partial E_{in}}{\partial \rho_{p_1}} \frac{\partial \hat{\rho}_{p_1}}{\partial \phi_{p_1}} \\
& = 2\alpha_1 \rho_{H_2} \left(\frac{|\phi_{p_1}(x, y, z, t)|}{2m_e + 2m_p} \right) |\phi_{A_1}(y, z, t)|^2 \rho_{H_2} \\
& - \beta_1 \left(\frac{\phi_{p_1}(x, y, z, t)}{2m_e + 2m_p} \right) |\phi_{A_1}(y, z, t)|^2 \rho_{H_2},
\end{aligned} \tag{97}$$

and

$$\begin{aligned}
 & \frac{\partial E_{in}}{\partial \rho_{p_2}} \frac{\partial \hat{\rho}_{p_2}}{\partial \phi_{p_2}} \\
 = & 2\alpha_1 \rho_{H_2} \left(\frac{|\phi_{p_2}(x, y, z, t)|}{2m_e + 2m_p} \right) |\phi_{A_2}(y, z, t)|^2 \rho_{H_2} \\
 & - \beta_1 \left(\frac{\phi_{p_2}(x, y, z, t)}{2m_e + 2m_p} \right) |\phi_{A_2}(y, z, t)|^2 \rho_{H_2}. \tag{98}
 \end{aligned}$$

Summing up the last previous equations and integrating them in x, y and recalling that

$$\begin{aligned}
 & (C_v)_{H_2} \rho_{H_2} T_{H_2} \\
 = & \frac{1}{2} c \rho_{e_1}(z, t) \sqrt{c^2 - g_{jk}^{e_1} \frac{\partial (X_{H_2})_j}{\partial t} \frac{\partial (X_{H_2})_k}{\partial t}} \sqrt{-g^{e_1}} |\det X'_{H_2}| \\
 & + \frac{1}{2} c \rho_{p_1}(z, t) \sqrt{c^2 - g_{jk}^{p_1} \frac{\partial (X_{H_2})_j}{\partial t} \frac{\partial (X_{H_2})_k}{\partial t}} \sqrt{-g^{p_1}} |\det X'_{H_2}| \\
 & + \frac{1}{2} c \rho_{e_2}(z, t) \sqrt{c^2 - g_{jk}^{e_2} \frac{\partial (X_{H_2})_j}{\partial t} \frac{\partial (X_{H_2})_k}{\partial t}} \sqrt{-g^{e_2}} |\det X'_{H_2}| \\
 & + \frac{1}{2} c \rho_{p_2}(z, t) \sqrt{c^2 - g_{jk}^{p_2} \frac{\partial (X_{H_2})_j}{\partial t} \frac{\partial (X_{H_2})_k}{\partial t}} \sqrt{-g^{p_2}} |\det X'_{H_2}|, \tag{99}
 \end{aligned}$$

we obtain

$$-(C_v)_{H_2} \rho_{H_2} T_{H_2} + C_1 + \left(\frac{P_{H_2}}{\rho_{H_2}} + B \right) \rho_{H_2} = 0, \tag{100}$$

where,

$$B = \frac{\partial J}{\partial \rho_{H_2}} - \frac{\partial J_S}{\partial \rho_{H_2}} + \frac{\partial E_{in}}{\partial \rho_{H_2}} + \frac{\partial J_{Aux_{30}}}{\partial \rho_{H_2}} + \frac{\partial J_{Aux_{34}}}{\partial \rho_{H_2}} + \frac{\partial J_{Aux_{11}}}{\partial \rho_{H_2}},$$

so that

$$\begin{aligned}
 B = & \frac{1}{2} \mathbf{v}_{H_2} \cdot \mathbf{v}_{H_2} + g(X_{H_2})_3 + \alpha_1 \rho_{H_2} - \beta_1 + \hat{K}_{H_2} T_{H_2} \left(\ln \left(\frac{\rho_{H_2}}{\rho} \right) - \omega_{H_e} \right) \\
 & + \frac{\partial J_{Aux_{30}}}{\partial \rho_{H_2}} + \frac{\partial J_{Aux_{34}}}{\partial \rho_{H_2}} + \frac{\partial J_{Aux_{11}}}{\partial \rho_{H_2}}, \tag{101}
 \end{aligned}$$

and

$$\begin{aligned}
C_1 = & \hat{\rho}_{e_1} \mathbf{v}_{e_1} \cdot \mathbf{v}_{H_2} / \sqrt{1 - \frac{v_{e_1}^2}{c^2}} \\
& - \hat{\rho}_{e_1} \mathbf{v}_{e_1} \cdot \mathbf{A} + K_1 V(z, t) \hat{\rho}_{e_1} \\
& + 2E_1(y, z, t) |\phi_{e_1}|^2 + \frac{\partial E_{in}}{\partial \rho_{e_1}} \hat{\rho}_{e_1} \\
& + \hat{\rho}_{p_1} \mathbf{v}_{p_1} \cdot \mathbf{v}_{H_2} / \sqrt{1 - \frac{v_{p_1}^2}{c^2}} \\
& - \hat{\rho}_{p_1} \mathbf{v}_{p_1} \cdot \mathbf{A} + K_1 V(z, t) \hat{\rho}_{p_1} \\
& + E_5(y, z, t) |\phi_{p_1}|^2 + \frac{\partial E_{in}}{\partial \rho_{p_1}} \hat{\rho}_{p_1} + \hat{\rho}_{e_2} \mathbf{v}_{e_2} \cdot \mathbf{v}_{H_2} / \sqrt{1 - \frac{v_{e_2}^2}{c^2}} \\
& - \hat{\rho}_{e_2} \mathbf{v}_{e_2} \cdot \mathbf{A} + K_1 V(z, t) \hat{\rho}_{e_2} \\
& + 2E_1(y, z, t) |\phi_{e_2}|^2 + \frac{\partial E_{in}}{\partial \rho_{e_2}} \hat{\rho}_{e_2} \\
& + \hat{\rho}_{p_2} \mathbf{v}_{p_2} \cdot \mathbf{v}_{H_2} / \sqrt{1 - \frac{v_{p_2}^2}{c^2}} \\
& - \hat{\rho}_{p_2} \mathbf{v}_{p_2} \cdot \mathbf{A} + K_1 V(z, t) \hat{\rho}_{p_2} \\
& + E_7(y, z, t) |\phi_{p_2}|^2 + \frac{\partial E_{in}}{\partial \rho_{p_2}} \hat{\rho}_{p_2}.
\end{aligned} \tag{102}$$

Now denoting

$$C_3 = \frac{\partial J_{Aux_{30}}}{\partial \rho_{H_2}} + \frac{\partial J_{Aux_{34}}}{\partial \rho_{H_2}} + \frac{\partial J_{Aux_{11}}}{\partial \rho_{H_2}},$$

we obtain

$$B = \frac{1}{2} \mathbf{v}_{H_2} \cdot \mathbf{v}_{H_2} + g(X_{H_2})_3 + \alpha_1 \rho_{H_2} - \beta_1 + \hat{K}_{H_2} \frac{T_{H_2}}{\rho} \left(\ln \left(\frac{\rho_{H_2}}{\rho} \right) - \omega_{H_e} \right) + C_3.$$

From such expressions for C_1 , C_3 and from (100), we have got

$$\begin{aligned}
& \frac{P_{H_2}}{\rho_{H_2}} + \frac{1}{2} \mathbf{v}_{H_2} \cdot \mathbf{v}_{H_2} + g(X_{H_2})_3 \\
& + \alpha_1 \rho_{H_2} - \beta_1 + \hat{K}_{H_2} \frac{T_{H_2}}{\rho} \left(\ln \left(\frac{\rho_{H_2}}{\rho} \right) - \omega_{H_e} \right) + C_3 \\
= & (C_v)_{H_2} T_{H_2} - \frac{C_1}{\rho_{H_2}}.
\end{aligned} \tag{103}$$

Thus, we have obtained the following equation

$$\begin{aligned}
 & P_{H_2} + \frac{1}{2} \rho_{H_2} \mathbf{v}_{H_2} \cdot \mathbf{v}_{H_2} + g \rho_{H_2} (X_{H_2})_3 \\
 = & C_{v_{H_2}} \rho_{H_2} T_{H_2} - \alpha_1 \rho_{H_2}^2 + \left(\beta_1 + \hat{K}_{H_2} T_{H_2} \frac{\omega_{H_e}}{\rho} \right) \rho_{H_e} \\
 & - \hat{K}_{H_2} T_{H_2} \left(\ln \left(\frac{\rho_{H_2}}{\rho} \right) \right) \frac{\rho_{H_e}}{\rho} - C_1 - C_3 \rho_{H_2}.
 \end{aligned} \tag{104}$$

In summary, we have obtained the partial approximate Bernoulli-interacting-gas equation,

$$\begin{aligned}
 & P_{H_2} + \frac{\rho_{H_2}}{2} \mathbf{v}_{H_2} \cdot \mathbf{v}_{H_2} + \rho_{H_2} g (X_{H_2})_3 \\
 = & K_3 \rho_{H_2} T_{H_2} - \alpha_1 \rho_{H_2}^2 + \left(\beta_1 + \hat{K}_{H_2} T_{H_2} \frac{\omega_{H_e}}{\rho} \right) \rho_{H_e} \\
 & - \hat{K}_{H_2} T_{H_2} \left(\ln \left(\frac{\rho_{H_2}}{\rho} \right) \right) \frac{\rho_{H_e}}{\rho} + D_1,
 \end{aligned} \tag{105}$$

for an appropriate function D_1 and an appropriate $K_3 > 0$ obtained through equation (104).

Moreover, from the variation of J_{total} in $\mathbf{v}_{H_2}$, we obtain

$$\rho_{H_2} \mathbf{v}_{H_2} + E_{17} + \nabla(\hat{P} \rho_{H_2}) + C_5 = \mathbf{0},$$

where

$$\begin{aligned}
 C_5 = & \frac{\rho_{e_1}}{\sqrt{1 - \frac{v_{e_1}^2}{c^2}}} \mathbf{v}_{e_1} + \frac{\rho_{e_2}}{\sqrt{1 - \frac{v_{e_2}^2}{c^2}}} \mathbf{v}_{e_2} \\
 & \frac{\rho_{p_1}}{\sqrt{1 - \frac{v_{p_1}^2}{c^2}}} \mathbf{v}_{p_1} + \frac{\rho_{p_2}}{\sqrt{1 - \frac{v_{p_2}^2}{c^2}}} \mathbf{v}_{p_2} \\
 & + \frac{\partial J_{Aux_{34}}}{\partial \mathbf{v}_{H_2}} + \frac{\partial J_{Aux_{11}}}{\partial \mathbf{v}_{H_2}},
 \end{aligned} \tag{106}$$

$$\frac{\partial J_{Aux_{34}}}{\partial \mathbf{v}_{H_2}} = -\nabla_z (E_{41}(z, t) P_{H_2}),$$

and $\frac{\partial J_{Aux_{11}}}{\partial \rho_{H_2}}$ is related to the following variation,

$$\delta J_{Aux_{11}}(\mathbf{v}_{H_2}; \varphi) = \int_0^T E_{15}(t) \left(- \int_0^t \int_{\Omega} \rho_{H_2} \varphi(y, \tau) \cdot \mathbf{n} dS d\tau \right) dt,$$

$\forall \varphi \in C^\infty(\Omega \times [0, T]; \mathbb{R}^3)$, which just generates a boundary condition for $E_{15}(t)$.

The variation of J_{total} in $\mathbf{r}_{H_2}$, stands for

$$-\rho_{H_2} \mathbf{g} + \frac{dE_{17}}{dt} + C_7 = 0,$$

where

$$C_7 = \frac{\partial J_{Aux_{30}}}{\partial \mathbf{r}_{H_2}} + \frac{\partial \left(\sum_{j=1}^4 E_{C_j} \right)}{\partial \mathbf{r}_{H_2}},$$

where such explicit expressions may be obtained similarly as above indicated.

Joining the pieces we have got

$$\rho_{H_2} \mathbf{g} + \frac{d(\rho_{H_2} \mathbf{v}_{H_2})}{dt} + \frac{d(\nabla(\hat{P} \rho_{H_2}))}{dt} - \frac{dC_5}{dt} - C_7 = 0,$$

so that

$$\frac{\partial(\rho_{H_2} \mathbf{v}_{H_2})}{\partial t} + \frac{\partial(\rho_{H_2} \mathbf{v}_{H_2})}{\partial (X_{H_2})_j} \frac{\partial (X_{H_2})_j}{\partial t} + \nabla P_{H_2} + \rho_{H_2} \mathbf{g} = \frac{dC_5}{dt} + C_7 \equiv C_9.$$

This just an approximate version of the well known Euler system.

Moreover, from the variation of J_{total} in $\hat{P}$, provide us,

$$\begin{aligned} & \frac{d\rho}{dt} + \rho_{H_2} \operatorname{div} \mathbf{v}_{H_2} + \rho_{H_a^+} \operatorname{div} \mathbf{v}_{H_a^+} \\ & + \rho_{H_b^+} \operatorname{div} \mathbf{v}_{H_b^+} + \rho_{e_3} \operatorname{div} \mathbf{v}_{e_3} + \rho_{e_4} \operatorname{div} \mathbf{v}_{e_4} + C_8 = 0, \end{aligned} \quad (107)$$

where

$$C_8 = \frac{\partial J_{Aux_{14}}}{\partial P} \frac{\partial P}{\partial \hat{P}}.$$

Hence, through the Eulerian identification

$$(X_{H_2})_k(y, t) \approx x_k, \quad \forall k \in \{1, 2, 3\},$$

we have obtained the following macroscopic system,

1. Euler type Equation:

$$\frac{\partial(\rho_{H_2} \mathbf{v}_{H_2})}{\partial t} + \frac{\partial(\rho_{H_2} \mathbf{v}_{H_2})}{\partial x_j} (\mathbf{v}_{H_2})_j + \nabla P_{H_2} + \rho_{H_2} \mathbf{g} = C_9,$$

2. Continuity type equation:

$$\begin{aligned} & \frac{d\rho}{dt} + \rho_{H_2} \operatorname{div} \mathbf{v}_{H_2} + \rho_{H_a^+} \operatorname{div} \mathbf{v}_{H_a^+} \\ & + \rho_{H_b^+} \operatorname{div} \mathbf{v}_{H_b^+} + \rho_{e_3} \operatorname{div} \mathbf{v}_{e_3} + \rho_{e_4} \operatorname{div} \mathbf{v}_{e_4} + C_8 = 0, \end{aligned} \quad (108)$$

3. A Temperature type equation:

$$\begin{aligned} & \rho_{H_2}(C_v)_{H_2} \frac{dT_{H_2}}{dt} + \rho_{H_a^+}(C_v)_{H_a^+} \frac{dT_{H_a^+}}{dt} \\ & + \rho_{H_b^+}(C_v)_{H_b^+} \frac{dT_{H_b^+}}{dt} + \rho_e(C_v)_e \frac{dT_e}{dt} \\ = & K_{H_2} \nabla^2 T_{H_2} + K_{H_a^+} \nabla^2 T_{H_a^+} + K_{H_b^+} \nabla^2 T_{H_b^+} + K_e \nabla^2 T_e \\ & - P_{H_2} \operatorname{div} \mathbf{v}_{H_2} - P_{H_a^+} \operatorname{div} \mathbf{v}_{H_a^+} - P_{H_b^+} \operatorname{div} \mathbf{v}_{H_b^+} \\ & - P_{e_3} \operatorname{div} \mathbf{v}_{e_3} - P_{e_4} \operatorname{div} \mathbf{v}_{e_4} + \frac{dE_S^M}{dt}. \end{aligned} \quad (109)$$

4. A Bernoulli-interacting-gas type equation:

$$\begin{aligned} & P_{H_2} + \frac{\rho_{H_2}}{2} \mathbf{v}_{H_2} \cdot \mathbf{v}_{H_2} + \rho_{H_2} g(X_{H_2})_3 \\ = & K_3 \rho_{H_2} T_{H_2} - \alpha_1 \rho_{H_2}^2 + \left(\beta_1 + \hat{K}_{H_2} T_{H_2} \frac{\omega_{H_e}}{\rho} \right) \rho_{H_e} \\ & - \hat{K}_{H_2} T_{H_2} \left(\ln \left(\frac{\rho_{H_2}}{\rho} \right) \right) \frac{\rho_{H_e}}{\rho} + D_1, \end{aligned} \quad (110)$$

for an appropriate function D_1 and an appropriate $K_3 > 0$.

Remark 6.2. We highlight the functions C_5, C_7, C_8 and C_9 may be exactly obtained from the exact concerning variations of J_{total} .

Finally, we also emphasize similar results may be obtained for $P_{H_a^+}, P_{H_b^+}, P_{e_3}$ and P_{e_4} .

The objective of this section is complete.

7 Conclusion

In this article, we have developed a variational formulation for a hydrogen molecule ionization chemical reaction.

In summary, we have obtained a functional such that the variation comprises a set of partial differential equations intended to mathematically model such an ionization process.

Finally, we highlight our main results include approximate Bernoullian-interacting-gas equations, which in some sense, make the role of the standard ideal gas and related equations in the contemporary literature in fluid mechanics.

References

- [1] F.S. Botelho, A Variational Formulation for Modeling a Fluid Motion in an Euler-Bernoullian Context: A Detailed Development. *The Journal of Engineering*, Vol 2025 (1), 2025.
<https://doi.org/10.1049/tje2.70097>
- [2] P. Constantin, C. Foias. *Navier-Stokes equation*, University of Chicago Press, Chicago, 1989.
- [3] C. De Lellis C, E. Brué, D. Albritton, M. Colombo, V. Giri, M. Janisch and H. Kwon. Instability and Non-uniqueness for the 2D Euler Equations, after M. Vishik (AMS-219) Volume 219 in the series *Annals of Mathematics Studies*, Princeton University Press, New Jersey, 2024.
<https://doi.org/10.1515/9780691257846>
- [4] M. Hamouda M, D. Han , C.-Y. Jung, R. Temam. Boundary layers for the 3D primitive equations in a cube: the zero-mode, *Journal of Applied Analysis and Computation*. 2018; 8, No. 3, (873-889), DOI:10.11948/2018.873.
- [5] A. Giorgini, A. Miranville, R. Temam. Uniqueness and regularity for the Navier-Stokes-Cahn-Hilliard system, *SIAM J. of Mathematical Analysis (SIMA)*.2019; 51, 3, (2535-2574), <https://doi.org/10.1137/18M1223459>.
- [6] C. Foias, R.M. Rosa, R. Temam. Properties of stationary statistical solutions of the three-dimensional Navier-Stokes equations, *J. of Dynamics and Differential Equations*, Special issue in memory of George Sell. 2019; 31, 3, 1689-1741, <https://doi.org/10.1007/s10884-018-9719-2>.
- [7] R. Temam. *Navier-Stokes Equations*, AMS Chelsea, reprint (2001).
- [8] Tannehill J C, Anderson D A, Pletcher R H. *Computational Fluid Mechanics and Heat Transfer*, 2nd edn., Taylor and Francis, Philadelphia, PA, 1997.

- [9] J.C. Strikwerda. finite difference schemes and partial differential equations, second edition Philadelphia, SIAM, 2004.
- [10] F.S. Botelho. "Approximate numerical procedures for the Navier-Stokes system through the generalized method of lines" *Nonlinear Engineering*, vol. 13, no. 1, 2024, pp. 20220376. <https://doi.org/10.1515/nleng-2022-0376>
- [11] F. Botelho. Existence of solution for the Ginzburg-Landau system, a related optimal control problem and its computation by the generalized method of lines, *Applied Mathematics and Computation*, 2012; 218 (11976-11989).
- [12] F.S. Botelho. An approximate proximal numerical procedure concerning the generalized method of lines. *Mathematics* 2022, 10(16), 2950; <https://doi.org/10.3390/math10162950>.
- [13] F. Botelho. *Functional Analysis and Applied Optimization in Banach Spaces*, (Springer Switzerland, 2014).
- [14] F.S. Botelho. *Functional analysis, calculus of variations and numerical methods in physics and engineering*. Boca Raton, Florida, USA CRC Taylor and Francis; 2020.
- [15] F.S. Botelho. *Advanced Calculus and its Applications in Variational Quantum Mechanics and Relativity Theory*, CRC Taylor and Francis, Florida, 2021.
- [16] S. Sheng and Z. Shao, Concentration of mass in the pressureless limit of the Euler equations of one-dimensional compressible fluid flow, *Nonlinear Analysis, Real world applications*, 52, (2020), 103039. <https://doi.org/10.1016/j.nonrwa.2019.103039>
- [17] R.A. Adams and J.F. Fournier. *Sobolev Spaces*, 2nd edn. (Elsevier, New York, 2003).
- [18] F.S. Botelho, *Duality Principles and Numerical Procedures for a Large Class of Non-Convex Models in the Calculus of Variations*. *Preprints* 2023, 2023020051. <https://doi.org/10.20944/preprints202302.0051.v95>